X-RAY STRUCTURAL STUDIES OF SOME GROUP VIII COMPOUNDS WITH CATALYTIC IMPLICATIONS

By
DOUGLAS ALLEN SULLIVAN

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To Jeanie

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KEY TO ABBREVIATIONS

LIPS	ligand-induced proton shift
H_2dmg	dimethylglyoxime
dmg	dimethylglyoxime dianion
Hdmg	dimethylglyoxime monoanion
H_2dmg_2	bis(dimethylglyoximate) with relative proton positions unspecified
sulfa	sulfanilamide
dhph	1,4-dihydrazinophthalazine
dhphpy	1,4-dihydrazinophthalazinebis(2-pyridinecarboxaldimine)
pyca	2-pyridinecarboxaldehyde
clan	4-chloroaniline
H_2dph	diphenylglyoxime
H_2mpg	methylphenylglyoxime
fph	pentafluorophenyl
cp	cyclopentadienyl anion
tpp	triphenylphosphine
an	aniline
4-FPYTSC	4-formylpyridinethiosemicarbazone

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By

Douglas Allen Sullivan

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X-ray structural investigations of compounds containing Group VIII metal atoms are presented. The compounds studied illustrate interatomic interactions which may be of importance in catalytic processes. The structures of metal-containing compounds were solved by locating the heavy atoms in Patterson functions and locating the remaining atoms in Fourier syntheses. The direct method of symbolic addition was used in the one, all light-atom case presented. Trial structures were refined by the method of least-squares.

The crystal structure of trans-chloro(dimethylglyoximato)(dimethylglyoxime)(4-chloroaniline)cobalt(III) illustrates an unusual ligand-induced proton shift. Both neutral and dianionic dimethylglyoxime groups are found in the complex and the 4-chloroaniline ligand is oriented over the dianionic dimethylglyoxime. The structure of trans-bis(dimethyl-

glyoximato)bis(4-chloroaniline)cobalt(III) chloride shows that complex to contain two monoatomic dimethylglyoxime ligands and the 4-chloroaniline ligands to be skewed relative to the diglyoxime ligands. The crystal structure of trans-chlorobis(diphenylglyoximato)(4-chloroaniline)cobalt-(III) is described. Trends in the structures of these compounds and in the previously reported structures of similar compounds are discussed. Ultraviolet and infrared spectra of these compounds are given.

The synthesis of a novel chelating ligand capable of binding two metal ions is described. The characterizations, including crystal structures, of its protonated form, 1,4-dihydrazinophthalazinebis(2-pyridiniumcarboxaldimine) nitrate dihydrate, and of a nickel complex, μ-chlorotetraaqua[1,4-dihydrazinophthalazinebis(2-pyridinecarboxaldimine)]dinickel-(II) chloride dihydrate, are presented. The planar ligand is shown to bind two nickel ions with a separation of 3.603 (1) Å. A chloride ion occupies a bridging site in the plane of the nickel atoms and the ligand. The magnetic moment per nickel atom of the chloride bridged complex was determined to be 2.74 B.M. at 40°C. The plausibility of structurally similar complexes mimicking the nitrogen-fixing enzyme nitrogenase is also discussed.

The X-ray crystal structures of 1-(π-cyclopentadienyl)-1-triphenylphosphine-2,3,4,5-tetrakis(pentafluorophenyl)cobaltole and 1-(π-cyclopentadienyl)-1-triphenylphosphine-2,3,4,5-tetrakis(pentafluorophenyl)rhodole are reported.

These compounds are viewed as stabilized intermediates in the catalyzed cyclization of acetylenes. In each case the metal atom forms a metallocycle by σ-bonding to the terminal carbons of a butadiene-like fragment. The π-bonding in the metallocycle appears to be delocalized.

CHAPTER 1
INTRODUCTION

Western civilization has demonstrated the efficiency-oriented phenomenon of expending large amounts of energy to find ways of requiring less human energy. This is evident in the evolution from animal trails to freeways and from muscle to sophisticated, high-energy machinery. On the molecular scale the more efficient path is provided by catalysts. As alchemists searched for the "philosopher's stone" many chemists have been seeking catalysts. The application of catalysis is now advancing through the development of an understanding of the mechanisms of catalytic processes.

Life processes are dependent upon chemical reactions controlled by enzymes. "It is not generally appreciated how little is understood about the mechanisms by which enzymes bring about their extraordinary and specific rate acceleration."[1] Investigation of enzymes should not only be fundamental in the understanding and maintenance of life processes but also should contribute to developing more efficient industrial processes.

Much of the investigation of enzymes has concerned the use of model compounds. "Model building and the application of material analogues are becoming increasingly important for the elucidation of fundamental problems of biochemical

structure and reactivity."[2] X-ray structural studies of enzyme models are important for the exploration of structure-activity relationships. Solid state studies of enzyme model compounds are of particular relevance because of the high degree of order the macromolecular enzymes themselves possess.

While electrostatic and hydrogen-bonding forces are usually considered the major binding forces in enzyme-substrate interactions, the strong charge-solvating and hydrogen-bonding ability of water tends to reduce the possibility of obtaining large binding energies from these forces. To explain the large binding energies found, "hydrophobic forces" are presumed to exist in these intermolecular interacions in aqueous solution.[3] The enthalpies of mixing of aromatic liquids with aliphatic liquids indicate that aromatic molecules prefer an aromatic environment.[4,5] "Stacking interactions" involving the π-systems of aromatic groups within the enzyme's protein structure may account for part of the "hydrophobic forces" and contribute to the orientation of the enzyme-substrate interaction.[3] The ligand-induced proton shift (LIPS) observed in $C\ell Co(H_2dmg)(dmg)(sulfa)$ [the key to abbreviations is given on page x] is an indication of the importance of this π-type interaction. A further examination of LIPS was undertaken and is presented in this work.

The design of enzyme models is often based on sparse structural information about the prosthetic group of the enzyme. Efforts to mimic the nitrogen-fixing enzyme nitrogenase

have been concerned with the metal to nitrogen bond. The probable binuclear nature of the enzyme's active site[6,7] has largely been ignored. The structures of a novel binucleating ligand and its nickel(II) complex are presented here as a first step in the construction of a new generation of models for nitrogenase.

When the mechanism of a chemical process is believed to be understood, stable compounds similar to the intermediates of the reaction may be prepared and examined to support the proposed mechanism. One proposed mechanism for the catalyzed cyclization of acetylenes would have a five-membered ring containing a metal atom and a cyclobutadiene fragment as one of the intermediates.[8-13] The first structure of such a stabilized intermediate containing a cobalt atom and the structure of the rhodium analog are presented in this study.

CHAPTER 2
SYNTHESIS AND CHARACTERIZATION

Synthesis

Crystals of all cobaloxime compounds were generously provided by R. C. Palenik* and were used without recrystallization.

M. D. Rausch and R. H. Gastinger synthesized the metallocycles containging cobalt[14] and rhodium.[15] They supplied well-formed crystals of those metallocycles for X-ray structural studies.

Unless otherwise indicated all solvents were reagent grade and were used without further purification. All preparations were carried out in air. All melting points were taken on a Mel-temp apparatus in open capillaries and are uncorrected.

The published method[16] was used to prepare dhph for succeeding experiments. To 6.40g (49.0 mmoles) 1,2-dicyanobenzene (98%; Aldrich Chemical Company, Milwaukee, Wisc.) in 12.5 ml 1,4-dioxane was added a mixture of 15.0 ml (ca. 250 mmoles) hydrazine hydrate (85%; Fisher Scientific Company, Fair Lawn, N. Y.) and 4.0 ml glacial acetic acid (reagent; Baker and Adamson, Morristown, N. J.). After being heated

*These complexes were prepared using standard procedures[17] with synthetic details to be published at a later date.

for three hours the mixture was cooled and the red product was collected (yield, ca. 40%). The decomposition temperature of 193°C was in agreement with the reported value.

A solution of 0.0955g (0.50 mmoles) of the previously prepared dhph in 40 ml absolute ethanol was added to a solution of 0.237g (1.0 mmoles) $NiC\ell_2 \cdot 6H_2O$ (reagent; Matheson, Coleman and Bell, Norwood, Ohio) and 0.095 ml (0.99 mmoles) pyca (99%; Aldrich) in 40 ml absolute ethanol. Upon slow, almost complete, evaporation in air of that solution olive green crystals of $[Ni_2C\ell(H_2O)_4(dhphpy)]C\ell_3 \cdot 2H_2O$ formed.

Analogous procedures were carried out replacing $NiC\ell_2 \cdot H_2O$ with $CoC\ell_2 \cdot 6H_2O$, $CuC\ell_2 \cdot 2H_2O$ (reagent; Fisher), $ZnC\ell_2$ (reagent; Mallinckrodt Chemical Works, St. Louis, Mo.) and $FeC\ell_2 \cdot 4H_2O$ (reagent; Matheson, Coleman and Bell) without success in obtaining a crystalline product. Similar procedures were followed with the addition of ca. 0.2 ml of 12 M hydrochloric acid (reagent, 38%; Baker and Adamson) to solutions of $CuC\ell_2 \cdot 2H_2O$ and $FeC\ell_2 \cdot 4H_2O$. Again, no suitable products were formed. Attempts to separate and recrystallize reaction products from water, water-ethanol, methanol and pyridine failed to give a crystalline product. When $CuC\ell_2$ was present, gas evolved from the reaction mixture.

Additional attempts were made to isolate complexes similar to $[Ni_2C\ell(H_2O)_4(dhphpy)]C\ell_3$ using dhph obtained by recrystallization from hot water of $H_2dhphSO_4$ (ICN·K and K Laboratories, Inc., Plainview, N. Y.) to which an equivalent

amount of KOH (certified A.C.S.; Fisher) had been added. Those attempts were unsuccessful.

The red-orange plates of $H_2dhphpy(NO_3)_2 \cdot 2H_2O$ used in crystallographic studies had been recrystallized from water. The crude product formed upon cooling a solution made by adding 0.190g (1.0 mmole) dhph in 20 ml warm water to a solution containing 0.583g (2.0 mmoles) $Ni(NO_3)_2 \cdot 6H_2O$ (reagent; Mallinckrodt) and 0.89 ml (9.4 mmoles) pyca in 10 ml warm water followed by drop-wise addition of nitric acid (reagent, 71%; Baker and Adamson) to a pH less than 1.

Also, $H_2dhphpy(NO_3)_2$ was prepared by first adding 1.90 ml (20.0 mmoles) pyca to a suspension of 2.878g (10.0 mmoles) $H_2dhphSO_4$ in 100 ml water. A brick-red solid formed upon addition of 1.11g (ca. 17 mmoles) KOH. After washing with water and drying in air, the brick-red solid was suspended in 100 ml of 95% ethanol and 1.30 ml (21 mmoles) of nitric acid were added. Small red-orange needles of $H_2dhphpy(NO_3)_2$ which decompose at 126°C were filtered, washed with ethanol, and then ether and air dried (yield 4.0g, 75%).

Freshly prepared hydrated metal hydroxides were reacted with $H_2dhphpy(NO_3)_2$ in methanol. Each of the metal hydroxides was filtered after adding 1 M KOH to aqueous solutions of $Ni(NO_3)_2 \cdot 6H_2O$, $Cu(NO_3)_2 \cdot 3H_2O$ (reagent; J. T. Baker Chemical Company, Phillipsburg, N. J.), $Fe(C\ell O_4)_2 \cdot 6H_2O$ (reagent; G. Frederick Smith Chemical Company, Columbus, Ohio) and $Zn(NO_3)_2 \cdot 6H_2O$ (reagent; Matheson, Coleman and Bell). After

the reaction mixtures were stirred until there was no further change in color, they were filtered and the filtrates were allowed to evaporate. Only the reaction with nickel(II) hydroxide produced a crystalline product. Attempts to recrystallize that maroon product from methanol, ethanol, ethanol-water, and 2-propanol did not yield crystals suitable for crystallographic studies.

Discussion of Characterization

The microananlyses recorded in Table 1 were performed by Galbraith Laboratories, Inc., Knoxville, Tennessee, for the dhphpy compounds and by Atlantic Microlab, Inc., Atlanta, Georgia, for the cobaloxime complexes. The calculated percentages of carbon, hydrogen, and nitrogen for the dhphpy compounds correlate well with the measured percentage. Two water molecules per molecule of dhphpy in each are indicated by the elemental analysis. This is confirmed in the structural determination. Similarly, the elemental analysis of $C\ell Co(H_2dmg)$(4-nitroaniline) is in agreement with the expected formula with two water molecules present. Based on the measured density and crystallographic data the molecular weight of $[Co(H_2dmg_2)$(4-methylaniline)$]C\ell$ should be 596. This is greater than its formula weight of 538.9 and the presence of molecules of solvation is expected. Three water molecules or one molecule of the ethanol solvent per formula could account for the difference. Neither of these possi-

Table 1

Elemental Analyses of Selected Compounds

	%C		%H		%N	
	found	calc.	found	calc.	found	calc.
$C\ell Co(H_2dmg_2)$(4-nitroaniline)$\cdot 2H_2O$	33.87	33.71	4.87	4.85	16.90	16.85
$[Co(H_2dmg_2)$(4-methylaniline)$_2]C\ell$	48.03	49.03	6.23	5.99	14.27	15.59
$\cdot 3H_2O$		44.56		6.46		14.17
$\cdot C_2H_5OH$		49.28		6.55		14.37
H_2dhphpy$(NO_3)_2\cdot 2H_2O$	45.36	45.29	4.12	4.18	26.10	26.40
$[Ni_2C\ell(H_2O)_4$(dhphpy)$]C\ell_3\cdot 2H_2O$	32.39	32.65	3.84	3.84	15.22	15.23

bilities is confirmed by the CHN analysis (see Table 1).

IR spectra of samples as mineral oil mulls between polished plates of fused sodium chloride were recorded on a Beckman Model IR10 grating spectrophotometer from 4000 to 500 cm^{-1}. The spectra were calibrated using the 1601.0 cm^{-1} absorption of a polystyrene film. IR spectra of selected compounds are reported in Table 2. The IR spectra of the bis(diglyoxime)cobalt(III) complexes with aniline derivatives exhibit many features of similar cobalt complexes with nitriles and isonitriles described by Batyr et al.[18] The spectra of the cobaloximes show the absorption assigned[18] to the C=N stretch between 1550 cm^{-1} and 1580 cm^{-1}. The absorptions associated[18] with the N-O band at ca. 1245 cm^{-1} and ca. 1095 cm^{-1} are present also. A weak absorption in the 1700-1800 cm^{-1} range appears in some of the spectra but with low resolution. Peaks in this region have been assigned[19] to the O···H-O bridge between the dioximate ligands. The presence of a symmetrical bridge has been suggested[20] to rationalize this low frequency.

Absorption spectra in the ultraviolet region were recorded on a Cary Model 15 spectrophotometer. Spectra of solutions were measured from 26.7 kK (375 mμ) to 47.6 kK (210 mμ) using the double beam method with the pure solvent as the reference. Solutions of the cobaloxime complexes in methanol (spectroquality; Matheson, Coleman and Bell) and solutions of the dhphpy compounds in 0.1 M hydrochloric

Table 2

Infrared Spectra[a] of Selected Compounds

$C\ell Co(H_2dmg_2)$-(dmg)(clan)	$C\ell Co(H_2dmg)$-(dmg)(sulfa)	$C\ell Co(H_2dmg_2)$-(4-nitroaniline)	$C\ell Co(H_2dpg_2)$-(clan)	$C\ell Co(H_2mpg_2)$-(clan)
3525(s)	3565(s)	3535(s)		
3425(s)		3410(s)	3400(m,b)	3480(m,b)
				3360(m)
	3195(s)			3165(m)
	3105(s)			3065(m)
2395(b,w)		2405(w,b)		
	2305(b,w)			
1907(w)	1930(w)			1897(w)
1778(b,w)	1780(b,w)			
1643(m)			1610(w)	
		1598(s)	1580(w)	1595(m)
1563(s)	1564(s)	1563(s)	1530(m)	1543(s)
1483(m)	1494(w)	1530(s)	1490(s)	1490(s)
			1445(s)	1445(s)
	1323(s)	1343(s)		
1242(s)	1244(s)	1244(s)	1292(m)	1263(s)
1203(s)		1200(m)		
1156(w)	1186(w)	1168(w)		

Table 2 - continued

$C\ell Co(H_2dmg)$-(dmg)(clan)	$C\ell Co(H_2dmg)$-(dmg)(sulfa)	$C\ell Co(H_2dmg_2)$-(4-nitroaniline)	$C\ell Co(H_2dpg_2)$-(clan)	$C\ell Co(H_2mpg_2)$-(clan)
	1152(s)			
1085(s)	1084(s)	1088(s)	1130(s)	1138(m)
				1085(w)
			1013(m)	1007(s)
973(b)	972(m)	971(m)		958(m)
	922(m)		920(w)	
	837(m)	858(s)	885(s)	
825(m)	824(m)	818(w)	823(w)	825(m)
		798(w)		
			757(w)	780(m)
742(m)		743(m)	730(s)	733(s)
705(m)		686(m)	685(s)	685(s)
645(w)	670(m)			

[a]Each column contains the respective absorption peaks (cm^{-1}) and the relative intensity (s, strong; m, moderate; w, weak; b, broad).

Table 2 - extended

[Co(Hdmg)$_2$-(clan)$_2$]Cℓ	[Co(H$_2$dmg$_2$)-(4-methylaniline)$_2$]Cℓ	[Ni$_2$Cℓ(H$_2$O)$_4$-(dhphpy)]Cℓ_3	H$_2$dhphpy-(NO$_3$)$_2\cdot$2H$_2$O
	3420(m,b)	3280(s,b)	3460(s,b)
			2050(w,b)
3125(s)			1750(w,b)
		1620(m)	1609(s)
2415(w)	2400(w,b)	1517(s)	1552(s)
2380(w)		1465(s)	
1892(w)		1380(s)	1290(s)
1785(b,w)		1296(w)	
	1638(w)	1285(w)	
1612(m)	1600(s)	1260(w)	1168(w)
1582(s)	1570(s)	1224(m)	
1493(s)	1506(s)	1137(s)	1141(m)
			1115(s)
		1096(w)	
1234(s)	1228(s)		1057(m)
1205(s)	1197(m)	1010(w)	950(w)
	1168(w)	912(w)	914(w)

Table 2 - extended - continued

$[Co(Hdmg)_2(clan)_2]C\ell$	$[Co(H_2dmg_2)$-(4-methylaniline)$_2]C\ell$	$[Ni_2C\ell(H_2O)_4(dhphpy)]C\ell_3$	$H_2dhphpy(NO_3)_2\cdot 2H_2O$
		865(w)	870(w)
1083(s)	1076(s)	824(w)	
		768(m)	775(m)
1008(m)	1013(m)		758(s)
967(m)	968(m)		
819(m)			
805(m)	808(m)		
735(m)	743(m)		
700(m)	701(w)		
647(m)			

acid were used. The UV spectra are reported in Table 3.

The UV spectra of all these compounds are dominated by intense charge transfer bands. Yamano *et al.*[21] report three bands in this region for compounds of the formula $[Co(H_2dmg_2)-A_2]$ where A is an aniline derivative. These three bands are present in $[Co(Hdmg)_2(clan)_2]C\ell$ and $[Co(H_2dmg_2)(4\text{-methylaniline})_2]C\ell$. The band between 25.0 and 27.5 kK (400 to 360 mμ) was assigned[21] to the charge transfer from the aniline ligand to the cobalt ion. In agreement with this assignment the band for the complex of the more basic 4-methylaniline at 27.6 kK is lower in frequency than that for the analogous complex of clan at 28.9 kK. The band near 33.0 kK (300 mμ) was assigned[21] to the charge transfer from the cobalt ion to the dioximate ligand. The band near 40.0 kK (250 mμ) was assigned[21] to the intra-Hdmg $\pi \rightarrow \pi^*$ transition.

The UV spectra of cobaloxime complexes with a chloride ligand *trans* to a substituted aniline show three bands, also. One band is between 27.0 and 33.0 kK (370 to 300 mμ). The other bands lie near 39.0 kK (255 mμ) and 43.0 kK (230 mμ). No assignments have been made for these three bands.

The charge transfer spectrum of a solution of $[Ni_2C\ell(H_2O)_4(dhphpy)]C\ell_3 \cdot 2H_2O$ in 0.1 M $HC\ell$ exhibits the same absorptions as that of a solution of $H_2dhphpy(NO_3)_2$ in 0.1 M $HC\ell$. The intense bands at 25.4, 32.7, and 37.3 kK (395, 305, and 268 mμ) are presumably due to the aromatic system of the ligand.

Table 3

Ultraviolet Spectra[a,b] of Selected Compounds

$[Co(Hdmg)_2(clan)_2]C\ell$	28.9(16000)	[32.7]	39.7(21000)
$[Co(H_2dmg_2)$(4-methylaniline)$_2]C\ell$	27.6(11000)	32.8(7400)	39.7(16000)
$C\ell Co(H_2dmg)(dmg)(clan)$	32.7(9200)	39.5(24000)	44.8(24000)
$C\ell Co(H_2mpg_2)(clan)$	31.1(7300)	39.8(27000)	[44.1]
$C\ell Co(H_2dpg_2)(clan)$	29.7(12000)	37.6(43000)	42.4(42000)
$C\ell Co(H_2dmg_2)$(4-nitroaniline)	27.2(20000)	[39.6]	42.9(33000)
$H_2dhphpy(NO_3)_2 \cdot 2H_2O$	25.4(5600)	32.8(4600)	37.3(4600)
$[Ni_2C\ell(H_2O)_4(dhphpy)]C\ell_3 \cdot 2H_2O$	25.4(25000)	32.7(20000)	37.3(20000)

[a]The compound name is followed by the absorption frequencies (kK) with the extinction coefficients in parentheses.

[b]Frequencies listed in square brackets are for poorly resolved peaks.

The magnetic moment per nickel atom of $[Ni_2C\ell(H_2O)$-(dhphpy)$]C\ell_3$ was determined to be 2.74 B.M. at 40°C. Data for this calculation[22,23] were obtained using a Varian A-60A Analytical NMR Spectrometer and aqueous solutions containing 2% by volume t-butanol as the indicator. This magnetic moment is in agreement with those of binuclear complexes of nickel reported by Ball and Blake.[24] Their complexes of the general formula $[Ni(dhph)]_2X_4 \cdot nH_2O$ (X = $C\ell$, Br, or I) had room temperature effective magnetic moments ranging from 2.79 to 2.89 B.M. As in the case of $[Ni(dhph)]_2X_4 \cdot nH_2O$, where two Ni^{2+} ions are bridged by a conjugated system, spin-spin interaction is indicated in $[Ni_2C\ell(H_2O)_4$(dhphpy)$]$-$C\ell_3 \cdot 2H_2O$.

CHAPTER 3
X-RAY DIFFRACTION EXPERIMENTAL

Except where noted in the text, the experimental methods described in this section were used in preliminary crystallographic examination, collection and processing of data, and refinement of trial structures.

Data obtained using precession and Weissenberg X-ray photographic techniques[25-27] were used in determining the preliminary space groups and cell constants. After centering fifteen intense reflections on a computer-controlled Syntex P$\bar{1}$ diffractometer and selecting an indexing consistent with preliminary photographs, accurate cell constants with estimated standard deviations were obtained from least-squares fittings of 2θ, Ω, χ, and ϕ for those reflections. In each case the orientation matrix for data collection and the unit cell volume with its standard deviation were derived from these data. The calculated density was in agreement with the density measured by the flotation method[28] except in the cases of the metal-containing heterocycles. The specific gravity of the flotation liquid was measured to ±0.01 with a precision hydrometer. Relevant crystallographic data for each of the compounds studied are given in Table 4.

The suitability of a crystal for data collection was determined by its physical shape and size, the ease with

Table 4

Crystallographic Data for A, $C\ell Co(H_2dmg)(dmg)(clan)\cdot 2H_2O$; B, $C\ell Co(H_2dpg_2)(clan)\cdot C_2H_5OH$; C, $[Co(Hdmg)_2(clan)_2]C\ell$; D, $H_2dhphpy(NO_3)_2\cdot 2H_2O$; E, $[Ni_2C\ell(H_2O)_4(dhphpy)]C\ell_3\cdot 2H_2O$; F, $C_4(fph)_4Co(cp)(tpp)$; G, $C_4(fph)_4Rh(cp)(tpp)$; H, $C\ell Co(H_2mpg_2)(clan)$; I, $C\ell Co(H_2dmg_2)$(4-nitroaniline)$\cdot 2H_2O$; J, $[Co(H_2dmg_2)$(4-methylaniline)$_2]C\ell$

Compound[a]	Formula	Crystal System	Systematic Absences	Space Group
A	$C_{14}C\ell_2CoH_{20}N_5O_4\cdot 2H_2O$	triclinic	none	$P\bar{1}$
B	$C_{34}C\ell_2CoH_{28}N_5O_4\cdot C_2H_5OH$	monoclinic	$h0\ell: h+\ell=2n+1$	$P2_1/n$
C	$C_{20}C\ell_3CoH_{25}N_6O_4$	triclinic	none	$P\bar{1}$
D	$C_{20}H_{18}N_{10}O_6\cdot 2H_2O$	monoclinic	$hk\ell: h+k=2n+1$ $h0\ell: \ell=2n+1$	C2/c
E	$C_{20}C\ell_4H_{24}N_8Ni_2O_4\cdot 2H_2O$	monoclinic	$hk\ell: h+k=2n+1$ $h0\ell: \ell=2n+1$	C2/c
F	$C_{51}CoF_{20}H_{20}P\cdot ?$	triclinic	none	$P\bar{1}$
G	$C_{51}F_{20}H_{20}PRh\cdot ?$	triclinic	none	$P\bar{1}$
H*	$C_{24}C\ell_2CoH_{24}N_5O_4$	triclinic	none	P1 or $P\bar{1}$
I*	$C_{14}C\ell CoH_{20}N_6O_6\cdot 2H_2O$	orthorhombic	$hk0: h+\ell=2n+1$	Pmmn or $Pm2_1n(Pmn2_1)$
J*	$C_{22}C\ell CoH_{32}N_6O_4\cdot ?$	monoclinic	$h0\ell: \ell=2n+1$	P2/c or Pc

[a]Data for compounds marked with an asterisk were obtained from photographic techniques.

Table 4 - extended

Compound	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	Volume ($Å^3$)
A	7.494(3)	11.838(4)	13.758(6)	106.31(3)	91.25(3)	112.79(3)	1068.3(7)
B	15.363(13)	12.385(3)	18.535(13)	90	96.55(7)	90	3503(4)
C	6.386(4)	8.710(5)	12.719(5)	90.55(4)	105.16(4)	98.83(4)	673.9(6)
D	20.480(3)	11.166(2)	10.704(2)	90	102.99(2)	90	2385.0(8)
E	15.016(6)	15.527(7)	28.704(17)	90	115.78(3)	90	6027(5)
F	11.680(3)	14.008(4)	20.455(9)	114.08(3)	107.41(3)	106.72(2)	2572.9(1.7)
G	11.715(4)	14.015(6)	20.420(6)	114.07(3)	106.97(3)	107.28(3)	2574.3(1.5)
H*	7.95	13.26	13.75	98.1	102.7	105.9	1330
I*	21.66	13.68	14.97	90	90	90	4436
J*	13.2	11.2	19.9	90	110.6	90	2750

Table 4 - extended

Compound	Molecular Weight	Z	ρ calc. (g/cm^3)	ρ meas. (g/cm^3)	Crystal Dimensions (mm^3)	Radiation Used	μ (cm^{-1})
A	488.22	2	1.518	1.52	0.24x0.18x0.07	MoKα	11.2
B	746.54	4	1.415	1.43	0.18x0.20x0.05	MoKα	7.1
C	578.75	1	1.426	1.44	0.19x0.31x0.35	MoKα	10.0
D	530.46	4	1.477	1.47	0.34x0.31x0.18	MoKα	1.3
E	735.73	8	1.622	1.63	0.29x0.30x0.14	MoKα	18.1
F	1102.79	2	1.423	1.59	0.27x0.31x0.50	MoKα	4.9
G	1146.57	2	1.479	1.60	0.14x0.24x0.43	MoKα	4.6
H*	576.3	2	1.439	1.47			
I*	498.8	8	1.494	1.50			
J*	538.9	4	1.300	1.44			

Table 4 - extended

Compound	μr	2θ Range	K	No. of Unique Reflections	No. of Observed Reflections
A	~0.2	0-45	2.0	2807	2000
B	~0.1	0-45	1.5	4364	2017
C	~0.2	0-45	2.0	1771	1662
D	~0.04	0-45	2.0	1573	1093
E	~0.5	0-45	2.0	3981	2959
F	~0.1	0-45	2.0	6772	5479
G	~0.1	0-45	2.0	6766	5235

which the reflections were centered on the diffractometer, and the values of the refined cell constants with their estimated standard deviations compared to the cell constants obtained by photographic methods. All intensity measurements were made with a Syntex P$\bar{1}$ diffractometer at ambient temperature. All unique refelctions up to a limiting 2θ value were measured using a variable speed θ-2θ scan technique. The scan rate was determined from a fast three-second counting scan of the reflection peak and varied linearly from 1°/minute for counting rates of 150.0 c/sec. or less to 24°/minute for 1500.0 c/sec. or more. The intensity, I, was defined:

$$I = (\text{scan rate})\left[(\text{total scan counts}) - \frac{(\text{background counts})}{(\text{background to scan rate})}\right].$$

Peaks were scanned from 1° below $K\alpha_1$ to 1° above $K\alpha_2$. Measurements of the background count were made at the limits of each scan. The estimated standard deviation, σ(I), of each reflection was taken to be:

$$\sigma(I) = \left[(\text{total scan counts}) + \frac{(\text{background counts})}{(\text{background to scan ratio})^2}\right]^{1/2}.$$

For molybdenum radiation, the incident beam was monochromatized by a low order reflection of graphite. Any changes in the system were detected by measuring four standard reflections after each 96 intensity measurements.

A standardized data set was obtained by scaling the data to the initial value of the sum of the measured intensities of the standard reflections. The scaled in-

tensities of duplicate or equivalent reflections were averaged. Reflections with an intensity greater than $K\sigma(I)$, where K is given in Table 4, were considered reliable. The unreliable reflections with $I<K\sigma(I)$ were identified by a minus sign and not included in further steps of the structure solution. Corrections for Lorentz-polarization were of the form:

$$\frac{1}{Lp} = \frac{\sin 2\theta}{(1+\cos^2 2\theta)} .$$

To obtain a set of observed structure factors, F_{obs}'s, the monochromator was also assumed to be 50% perfect crystal and 50% mosaic crystal.

Scattering factors were obtained from Hanson, Herman, Lea, and Skillman;[29] Stewart, Davidson, and Simpson;[30] Doyle and Turner;[31] and are uncorrected for anomalous dispersion. The natural log of the scale factor and the overall temperature factor were initially estimated from a Wilson pilot.[32] The initial choice of a centric or acentric space group was made on the basis of calculated intensity statistics.[33]

In the case where molecules contained at least one heavy atom (Atomic Number $\geq$ 16) the approximate positional coordinates were determined using a Patterson function[34] of the form:

$$P(UVW) = \frac{2}{V} \sum_{h=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} |F(hkl)|^2 \cos 2\pi(hU+kV+lW) .$$

Using the location of the heavy atom(s) in a structure

factor calculation allowed a sufficient number of reflection phases, α(hkl)'s, to be assigned. The magnitude of the structure factor, $|F_{hkl}|$, and the phase may be defined by the following equations:[27]

$$A_{hkl} = \sum_j f_j \cos 2\pi(hx_j + hy_j + lz_j)$$

$$B_{hkl} = \sum_j f_j \sin 2\pi(hx_j + hy_j + lz_j)$$

$$|F_{hkl}| = (A^2_{hkl} + B^2_{hkl})^{1/2}$$

$$\alpha_{hkl} = \tan^{-1}(B_{hkl} / A_{hkl}),$$

where f_j is the scattering factor for atom j.

Additional atomic positions could then be determined through the use of Fourier syntheses[34] of the form:

$$(XYZ) = \frac{2}{V} \sum_{h=0}^{\infty} \sum_{k=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} |F_{hkl}| \cos 2\pi[(hX+kY+lZ)-\alpha_{hkl}].$$

The positional coordinates of atoms in the trial structure were estimated from the Fourier generated electron density map using a FORTRAN computer program, BOOTHIT1, written in the course of this work. A description and listing of BOOTHIT1 is contained in Appendix A. Alternate structure factor calculations and Fourier syntheses were repeated until all nonhydrogen atoms were located.

In the case of a compound not containing a heavy atom but having a centrosymmetric space group, the direct method of symbolic addition was used. The FORTRAN computer programs, FAME-MAGIC-LINK-SYMPL, developed by E. B. Fleischer, R. B.

K. Dewar, and A.L. Stone[35,36] were used to generate possible solutions to the phase problem. The programs first converted $|F_{obs}|$'s to normalized structure factors, E's, through the definitions:

$$(F_{absolute})^2 = \left(\frac{1}{K^2}\right)|F_{obs}|^2 \; e^{(T \sin \theta)/\lambda}$$

and

$$E^2 = (F_{absolute})^2/\varepsilon\sum_{i}^{N} f_i^2$$

where the scale factor, K, and the overall temperature factor, T, were generated by a Wilson plot; where ε was a symmetry factor applied to reflections in special zones; and where f_i's were the scattering factors for N atoms. The programs then assigned symbols representing the phases to six of the largest E's having the greatest number of interactions, i.e., for E_h and E_m there exists E_{h-m}. For such reflections the probability, p, that the phase of E_h is the same as $\sum_{m=0}^{N} (E_m E_{h-m})$ is given by:

$$p = 0.5 + 0.5 \tanh \left(\frac{\sigma_3}{\sigma_2 1.5}|E_h|\left|\sum_{m=0}^{N} E_m E_{h-m}\right|\right)$$

where

$$\sigma_n = \sum_{j=1}^{N} Z_j^n$$

with N being the number of atoms in the unit cell and Z_j being the atomic number of the j^{th} atom. The programs, when given minimum acceptable probability criteria, iteratively assigned relative signs to the phase symbols. Combinations of these

signed phase symbols were finally used in conjunction with their structure factors to generate E-maps. The positional coordinates of most nonhydrogen atoms were determined from one of these E-maps. Structure factor calculations and Fourier syntheses were used to refine the atomic positions and, as in the heavy atom case, to locate any previously unfound nonhydrogen atoms of the trial structure.

The trial structure was refined by least-squares minimization[34] of the function:

$$\text{Residual} = \Sigma\, w(||F_{obs}| - |F_{calc}||)^2$$

where

$$\sqrt{w} = |F_{obs}|/|F_{low}| \quad \text{for } |F_{obs}| < |F_{low}|$$

$$\sqrt{w} = 1.0 \quad \text{for } |F_{low}| \leq |F_{obs}| \leq |F_{high}|$$

and

$$\sqrt{w} = |F_{high}|/|F_{obs}| \quad \text{for } |F_{obs}| > |F_{high}|$$

F_{low} and F_{high} are constants given in Table 4. Prior to refinement, an overall scale factor was chosen such that the sum of F_{obs} equaled the sum of F_{calc}. Isotropic temperature factors were used in the first three cycles of refinement and then anisotropic temperature factors of the form:

$$\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}\ell^2 + \beta_{12}hk + \beta_{13}h\ell + \beta_{23}h\ell)]$$

were used. The reliability index, R, was defined by:

$$R = \frac{\Sigma||F_{obs}| - |F_{calc}||}{\Sigma|F_{obs}|}$$

Calculations were performed on an IBM 370/165 computer with programs written or modified by Dr. Gus J. Palenik, except where previously noted. The refinement of each structure is outlined in Table 5.

Table 5

Schemes of Refinement

Compound	R-index with all nonhydrogen atoms from Fourier synthesis	Refinement with isotropic thermal parameters		Refinement[a] with anisotropic thermal parameters	
		No. of cycles	R-index	No. of cycles	R-index
$C\ell Co(H_2dmg)(dmg)(clan)\cdot 2H_2O$	0.27	3	0.095	3	0.066
$C\ell Co(H_2dpg_2)(clan)\cdot C_2H_5OH$	0.229	3	0.132	3	0.093
$[Co(Hdmg)_2(clan)_2]C\ell$	0.255	3	0.141	6	0.056
$H_2dhphpy(NO_3)_2\cdot 2H_2O$	0.32	3	0.134	3*	0.076
$[Ni_2C\ell(H_2O)_4(dhphpy)]C\ell_3\cdot 2H_2O$	0.21	3	0.090	3	0.062
$C_4(fph)_4Co(cp)(tpp)$	0.26	3	0.137	9	0.077
$C_4(fph)_4Rh(cp)(tpp)$	0.168	3	0.105	9	0.065

[a]The block-diagonal approximation to the full matrix was used except where marked with an asterisk.

Table 5 - extended

Compound	Refinement[a] with hydrogen atoms included isotropically but not refined		Refinement[a] with hydrogen atoms refined isotropically		F_{low}	F_{high}
	No. of cycles	R-index	No. of cycles	R-index		
$C\ell Co(H_2dmg)(dmg)(clan)\cdot 2H_2O$	3	0.052	6	0.047	18.0	49.0
$C\ell Co(H_2dpg_2)(clan)\cdot C_2H_5OH$	3	0.087	9	0.075	55.0	145.0
$[Co(Hdmg)_2(clan)_2]C\ell$	3	0.038	9	0.033	4.5	12.0
$H_2dhphpy(NO_3)_2\cdot 2H_2O$	-	-	6	0.050	8.0	22.0
$[Ni_2C\ell(H_2O)_4(dhphpy)]C\ell_3\cdot 2H_2O$	6	0.048	-	-	32.0	86.0
$C_4(fph)_4Co(cp)(tpp)$	-	-	-	-	17.5	35.0
$C_4(fph)_4Rh(cp)(tpp)$	-	-	-	-	17.5	35.0

CHAPTER 4

AN INVESTIGATION OF LIGAND-INDUCED PROTON SHIFT: THE CRYSTAL AND MOLECULAR STRUCTURES OF TRANS-CHLORO(DIMETHYLGLYOXIMATO)-(DIMETHYLGLYOXIME)(4-CHLOROANILINE)COBALT(III) DIHYDRATE, TRANS-CHLOROBIS(DIPHENYLGLYOXIMATO)(4-CHLOROANILINE)COBALT(III) ETHANOLATE, AND TRANS-BIS(DIMETHYLGLYOXIMATO)BIS(4-CHLOROANILINE)COBALT(III) CHLORIDE.

The stability of bis(dimethylglyoxime)metal complexes has long been known and their importance in both qualitative and quantitative analysis has been widely recognized.[37,38] Metal complexes of Hdmg have been used to study the *trans*-effect[39] and the *trans*-influence[40,41] of various ligands in octahedral complexes. Since the structural determination of the B_{12} coenzyme the *trans*-bis(dimethylglyoxime)cobalt complexes have become of considerable interest.[42-44] Schrauzer[42] has stated that to be capable of mimicking B_{12} a complex is required only to have a cobalt ion in the presence of a strong-binding planar ligand. Because $Co(H_2dmg_2)$ complexes successfully mimic the reactions of a cobalt ion in the corrin ring and because they are synthetically expedient, complexes of $Co(H_2dmg_2)$ have been investigated extensively in solution as models for B_{12}.[45]

Until very recently there have been few structural data on $Co(H_2dmg_2)$ complexes.[40,41,46-52] Except for the work of Palenik *et al*.[46] no structural investigation has been made of the interaction between the axial ligand and the equatorial Hdmg ligands. This interaction may be of considerable consequence.

Although sulfonamides are potent inhibitors of carbonic anhydrase they do not form strong coordination bonds with transition metal ions. Therefore, an interaction of the aromatic ring of the sulfonamide with the carbonic anhydrase protein has been proposed[53] to make a large contribution to the observed stability of the carbonic anhydrase-sulfonamide complex. Since a cobalt atom can replace the zinc atom in carbonic anhydrase with only a 50% decrease in activity, complexes of Co(H_2dmg$_2$) may prove to be useful models for investigating the interaction of sulfonamides with carbonic anhydrase.

An apparent ligand-induced proton shift (LIPS) was observed[46] in CℓCo(H_2dmg$_2$)(sulfa) which should be formulated CℓCo(H_2dmg)(dmg)(sulfa). To investigate further the LIPS phenomena and to examine interligand interactions within this type of complex the determination of the structures of CℓCo-(H_2dmg)(dmg)(clan), [Co(Hdmg)$_2$(clan)$_2$]Cℓ, and CℓCo(H_2dmg$_2$)-(clan) was undertaken.

Structure Solution and Refinement for CℓCo(H_2dmg)(dmg)(clan)·2H_2O

The heavy atom method was used with the positions of the cobalt atom and of the ionic chloride ligand estimated from a sharpened Patterson function. The magnitude of the Patterson function for the Co to Cℓ vectors was of the same order as that for the Co to Co vector. The positions of the heavy atoms, therefore, appeared ambiguous and several combinations were used in Fourier syntheses to determine their actual lo-

cations. Successive Fourier syntheses then revealed the locations of all nonhydrogen atoms in the compound. Three cycles of full-matrix least-squares refinement with individual isotropic thermal parameters and then three cycles of least-squares refinement using the block approximation with individual anisotropic thermal parameters reduced R to 0.066. A difference Fourier synthesis then indicated the absence of additional nonhydrogen atoms and revealed the positions of all hydrogen atoms. An outline of the refinement is given in Table 5. The refinement was terminated after the parameter shifts for the nonhydrogen atoms were less than one-tenth of their corresponding estimated standard deviations.

The scattering factors for cobalt, chlorine, oxygen, nitrogen, and carbon were from Hanson et al.[29] while those for hydrogen were from Stewart et al.[30] A list of the observed and calculated structure factors has been published and is available.[46] The final positional and thermal parameters are given in Tables 6 and 7.

Structure Solution and Refinement for $C\ell Co(H_2dpg_2)(clan)\cdot C_2H_5OH$

The nonstandard space group $P2_1/n$ was chosen since the standard $P2_1/c$ space group would require a very large value for β. The position of the cobalt atom was estimated from a sharpened Patterson function. The location of atoms and the refinement proceeded as in the case of $C\ell Co(H_2dmg)(dmg)(clan)\cdot 2H_2O$. Two atoms, O(S1) and C(S1), of an apparent solvent mole-

Table 6
Final Atomic Parameters of Nonhydrogen Atoms for $C\ell Co(H_2dmg)$-(dmg)(clan)[a]

Atom	x	y	z	β_{11}	β_{22}
Co	19148(12)	36142(8)	21611(6)	1287(16)	454(7)
Cℓ(1)	-1353(2)	2445(1)	1882(1)	148(3)	65(2)
Cℓ(2)	8142(4)	10300(2)	3785(2)	512(9)	67(2)
O(11)	1633(7)	4573(4)	534(3)	305(13)	95(5)
O(12)	1742(6)	4621(4)	4260(3)	304(13)	89(5)
O(21)	2285(7)	2611(4)	3796(3)	314(13)	104(5)
O(22)	1944(7)	2468(4)	17(3)	298(13)	114(6)
N(1)	4821(7)	4589(5)	2375(3)	157(12)	93(6)
N(11)	1600(7)	4753(5)	1536(3)	179(12)	75(6)
N(12)	1693(7)	4792(4)	3347(3)	156(12)	58(5)
N(21)	2289(7)	2459(5)	2788(3)	191(13)	72(5)
N(22)	2144(7)	2398(5)	980(3)	168(12)	74(5)
C(11)	1403(8)	5758(6)	2145(5)	170(15)	67(7)
C(12)	1443(8)	5772(6)	3208(5)	168(15)	59(6)
C(13)	1247(10)	6794(6)	1785(5)	268(19)	85(8)
C(14)	1310(10)	6815(7)	4067(5)	281(20)	100(8)
C(21)	2584(9)	1516(6)	2201(17)	214(17)	66(7)
C(22)	2509(9)	1475(6)	1124(5)	164(15)	65(7)
C(23)	3010(14)	584(8)	2593(7)	530(32)	112(10)
C(24)	2779(12)	465(7)	277(6)	410(27)	121(10)
C(1)	5676(7)	5999(5)	2722(4)	96(13)	70(6)
C(2)	6105(9)	6655(6)	3753(5)	198(16)	71(7)
C(3)	6866(9)	7971(6)	4082(5)	221(17)	91(8)
C(4)	7201(10)	8629(6)	3382(6)	195(17)	73(7)
C(5)	6809(10)	7972(7)	2340(5)	237(19)	99(8)
C(6)	6047(9)	6644(6)	2005(5)	191(16)	82(7)
O(w1)	6682(7)	3785(5)	646(4)	264(13)	148(7)
O(w2)	6802(7)	3830(5)	3690(3)	276(13)	166(7)

[a]All values are x 10^4 except for Co which are x 10^5. The estimated standard deviations are given in parentheses. The temperature factors are of the form: $\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}\ell^2 + \beta_{12}hk + \beta_{13}h\ell + \beta_{23}k\ell)]$.

Table 6 - extended

β_{33}	β_{12}	β_{13}	β_{23}
276(4)	822(17)	219(13)	157(9)
53(1)	78(4)	25(3)	14(2)
138(2)	65(7)	46(7)	46(4)
36(3)	168(14)	7(9)	44(6)
32(3)	167(13)	70(9)	33(6)
41(3)	199(14)	74(10)	70(6)
30(3)	199(14)	31(9)	25(6)
37(3)	123(14)	29(10)	50(7)
35(3)	108(14)	24(10)	26(7)
35(3)	71(13)	30(9)	19(6)
41(3)	123(14)	41(10)	39(7)
35(3)	99(13)	21(10)	12(7)
53(4)	101(17)	25(13)	41(9)
51(4)	73(16)	30(13)	14(8)
76(5)	190(21)	-5(16)	55(10)
62(5)	214(22)	50(16)	-6(10)
56(4)	134(18)	47(14)	44(9)
60(5)	110(17)	52(13)	24(9)
102(7)	347(31)	148(24)	106(14)
73(6)	301(28)	87(20)	11(12)
44(4)	72(15)	23(11)	44(8)
47(4)	89(17)	4(13)	28(9)
42(4)	95(19)	4(14)	8(9)
82(6)	61(18)	23(16)	39(10)
69(5)	99(20)	83(16)	95(11)
52(4)	104(18)	56(13)	52(9)
80(4)	241(16)	102(11)	100(8)
53(3)	295(16)	20(10)	22(7)

Table 7

Final Parameters for the Hydrogen Atoms for $C\ell Co(H_2dmg)(dmg)$-(clan)[a]

Atom [Bonded to]	Distance	x	y	z	B
H(B1)[O(22)]	1.16(8)	153(10)	335(7)	17(5)	6.3(1.8)
H(B2)[O(21)]	1.13(8)	184(10)	345(7)	402(5)	6.7(1.8)
H(2)[C(2)]	0.89(5)	·591(7)	621(5)	420(4)	2.0(1.1)
H(3)[C(3)]	0.99(7)	726(10)	858(7)	478(5)	6.7(1.9)
H(5)[C(5)]	0.90(7)	709(10)	838(7)	187(5)	5.8(1.7)
H(6)[C(6)]	1.01(5)	568(7)	609(5)	127(4)	2.0(1.1)
H(7)[N(1)]	1.03(7)	522(10)	434(6)	166(5)	6.1(1.7)
H(8)[N(1)]	0.83(6)	518(9)	428(6)	278(5)	4.5(1.5)
H(11)[C(13)]	0.96(8)	243(11)	753(7)	212(6)	8.2(2.1)
H(12)[C(13)]	0.79(9)	37(11)	692(7)	203(6)	8.5(2.2)
H(13)[C(13)]	1.00(1)	102(10)	663(7)	103(5)	7.1(1.9)
H(14)[C(14)]	1.02(7)	46(9)	639(6)	453(5)	5.8(1.7)
H(15)[C(14)]	0.78(7)	62(9)	708(6)	388(5)	4.9(1.5)
H(16)[C(14)]	0.87(8)	228(11)	734(8)	456(6)	8.6(2.2)
H(21)[C(23)]	0.86(10)	414(12)	59(8)	248(6)	9.6(2.4)
H(22)[C(23)]	0.92(9)	239(12)	-21(8)	211(6)	9.3(2.4)
H(23)[C(23)]	0.97(9)	266(12)	52(8)	326(7)	9.8(2.5)
H(24)[C(24)]	1.03(9)	242(12)	44(8)	-46(7)	9.4(2.4)
H(25)[C(24)]	0.84(10)	396(12)	58(8)	29(6)	9.1(2.3)
H(26)[C(24)]	1.00(7)	210(10)	-38(7)	40(5)	5.9(1.7)
H(w1)[O(w1)]	0.70(8)	659(11)	319(7)	69(6)	7.2(2.0)
H(w1')[O(w1)]	0.80(13)	771(16)	438(11)	72(9)	15.2(3.7)
H(w2)[O(w2)]	0.79(7)	736(10)	420(7)	425(5)	6.6(1.8)
H(w2')[O(w2)]	0.71(7)	747(10)	371(6)	337(5)	6.0(1.8)

[a]The hydrogen atom is given followed by the atom to which it is bonded in brackets, the corresponding bond distance (in Å), the positional parameters with estimated standard deviations ($x\ 10^{+3}$), and the isotropic thermal parameter (in $Å^2$).

cule were located before refinement. The scheme of the refinement is outlined in Table 5.

Although the compound was crystallized from ethanol, difference Fourier syntheses at various stages of refinement failed to indicate the position of an additional atom in the solvent molecule. Because a large region of relative high electron density existing near C(S1) could be indicative of an atom with high disorder and because ethanol was the solvent, a molecule of ethanol was assumed to be present for the purposes of determining the formula, molecular weight, and density.

The cobalt, chlorine, oxygen, nitrogen, and carbon scattering factors were taken from Hanson et al.[29] and those for hydrogen from Stewart et al.[30] Table B-1 is a list of observed and calculated structure factors for $C\ell Co(H_2dpg_2)$-(clan). The final positional and thermal parameters are shown in Tables 8 and 9.

Structure Solution and Refinement for $[Co(Hdmg)_2(clan)_2]C\ell$

With one molecule per unit cell in the centric $P\bar{1}$ space group the cobalt atom and the chloride anion were required to lie on centers of symmetry. The sharpened Patterson function was in agreement with the chloride ion at 0½0 when the cobalt atom is placed at 000. The remaining atoms were located in a similar manner as in $C\ell Co(H_2dmg)(dmg)(clan)$. An outline of the refinement is given in Table 5.

Table 8

The Final Atomic Parameters for the Nonhydrogen Atoms of CℓCo $(H_2dpg)_2$(clan)[a]

Atom	x	y	z	β_{11}	β_{22}
Co	3339(1)	3017(2)	2961(1)	33(1)	58(1)
Cℓ(1)	3101(2)	4797(3)	3049(2)	45(2)	68(3)
Cℓ(2)	6313(4)	60(5)	1153(3)	96(4)	151(6)
O(11)	3953(5)	3496(7)	1583(4)	47(5)	82(9)
O(12)	4349(5)	2916(10)	4348(4)	41(5)	210(13)
O(21)	2763(6)	2628(8)	4340(4)	54(5)	130(11)
O(22)	2334(5)	3078(8)	1587(4)	42(5)	102(9)
N(1)	3495(6)	1461(9)	2903(6)	29(6)	97(12)
N(11)	4172(6)	3351(7)	2306(4)	41(6)	41(8)
N(12)	4368(7)	3168(9)	3660(5)	56(7)	78(11)
N(21)	2534(7)	2738(9)	3635(5)	50(6)	85(11)
N(22)	2312(6)	2882(9)	2294(4)	39(6)	62(9)
C(11)	4970(8)	3533(10)	2591(6)	24(7)	88(14)
C(12)	5080(8)	3361(11)	3373(6)	44(8)	101(15)
C(13)	5698(8)	3915(12)	2191(6)	38(8)	70(12)
C(14)	5956(9)	3431(11)	3862(7)	42(8)	82(14)
C(21)	1706(8)	2557(10)	3364(6)	46(8)	58(12)
C(22)	1575(7)	2672(10)	2562(5)	28(6)	66(12)
C(23)	1055(8)	2220(10)	3832(6)	54(8)	50(12)
C(24)	709(8)	2583(10)	2146(6)	52(8)	46(12)
C(1)	4167(8)	1048(11)	2436(6)	54(9)	46(11)
C(2)	5012(9)	858(11)	2798(7)	65(10)	65(14)
C(3)	5687(9)	544(11)	2387(8)	53(9)	62(13)
C(4)	5487(9)	448(11)	1654(8)	69(10)	53(13)
C(5)	4661(10)	592(13)	1341(7)	74(10)	123(18)
C(6)	3990(8)	883(11)	1733(7)	45(8)	67(13)
C(1A)	5975(8)	3387(11)	1614(7)	35(8)	92(15)
C(2A)	6642(9)	3760(13)	1251(7)	54(9)	111(16)
C(3A)	7077(8)	4683(12)	1485(7)	36(8)	97(15)
C(4A)	6831(9)	5248(13)	2052(8)	46(9)	108(15)
C(5A)	6157(9)	4877(12)	2413(7)	69(10)	93(15)

Table 8 - extended

β_{33}	β_{12}	β_{13}	β_{23}
19(0)	-7(3)	2(1)	-4(2)
40(1)	8(5)	11(3)	-13(4)
100(3)	71(9)	96(5)	-15(7)
21(3)	12(11)	6(6)	26(8)
16(3)	-17(16)	-8(6)	7(13)
20(3)	-35(13)	3(6)	8(9)
21(3)	-18(13)	-4(5)	12(10)
34(4)	-9(13)	7(8)	-15(12)
13(3)	23(11)	-6(6)	14(8)
26(4)	7(15)	-1(8)	7(12)
20(3)	-15(14)	6(7)	-21(11)
16(3)	-12(14)	13(6)	6(11)
23(4)	5(16)	16(9)	28(13)
18(4)	-5(18)	7(9)	0(13)
23(4)	20(17)	20(9)	23(14)
28(5)	-11(17)	-8(10)	5(13)
23(4)	4(15)	12(9)	-2(12)
15(4)	24(15)	-4(8)	7(11)
17(4)	-43(17)	3(8)	-9(12)
28(5)	26(16)	-1(10)	30(12)
30(5)	-5(18)	-18(10)	20(14)
36(6)	-17(19)	-7(11)	15(15)
45(6)	45(18)	4(12)	2(15)
46(6)	58(19)	40(12)	20(15)
37(6)	19(23)	44(12)	70(17)
33(5)	-69(17)	9(10)	-29(14)
39(5)	5(17)	31(10)	4(15)
29(5)	10(21)	22(11)	2(16)
45(6)	-12(19)	9(11)	46(16)
43(6)	-28(21)	30(11)	18(19)
32(5)	7(22)	11(11)	2(17)

Table 8 - continued

Atom	x	y	z	β_{11}	β_{22}
C(1B)	6675(9)	2815(14)	3687(7)	61(9)	113(16)
C(2B)	7444(9)	2801(13)	4142(7)	59(9)	89(15)
C(3B)	7498(9)	3363(15)	4781(7)	56(10)	189(23)
C(4B)	6828(9)	4051(16)	4937(7)	59(10)	207(22)
C(5B)	6047(10)	4094(14)	4476(7)	73(11)	148(19)
C(1C)	664(9)	1226(12)	3750(7)	66(10)	73(14)
C(2C)	20(9)	872(12)	4199(7)	66(10)	96(16)
C(3C)	-212(9)	1576(14)	4700(8)	32(8)	183(23)
C(4C)	184(9)	2563(12)	4813(7)	61(10)	112(17)
C(5C)	826(8)	2872(11)	4368(6)	60(8)	41(11)
C(1D)	593(9)	2121(12)	1437(6)	54(8)	83(14)
C(2D)	-224(9)	1992(14)	1046(7)	56(9)	116(16)
C(3D)	-951(9)	2410(12)	1345(7)	50(9)	105(17)
C(4D)	-888(8)	2847(12)	2044(7)	42(8)	77(14)
C(5D)	-69(8)	2975(12)	2447(6)	30(7)	63(12)
O(S1)	1418(9)	4904(10)	944(5)	190(13)	136(13)
C(S1)	1450(26)	4854(22)	182(12)	512(49)	196(30)

[a]All values are x 10^4. The estimated standard deviations are given in parentheses. The temperature factors are of the form: $\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}\ell^2 + \beta_{12}hk + \beta_{13}h\ell + \beta_{23}k\ell)]$.

Table 8 - continued - extended

β_{33}	β_{12}	β_{13}	β_{23}
39(6)	-11(22)	-24(11)	13(18)
39(5)	-24(21)	-4(11)	24(17)
32(5)	-59(24)	13(11)	-5(18)
18(5)	-47(26)	0(10)	-39(19)
28(5)	-90(25)	7(11)	0(18)
28(5)	-27(19)	-3(11)	-20(15)
28(5)	-24(21)	7(11)	13(16)
44(6)	-21(21)	-26(11)	-5(19)
26(5)	16(19)	26(10)	-10(14)
28(4)	-31(19)	-7(9)	8(14)
28(5)	-4(20)	7(10)	-16(16)
34(5)	13(23)	-34(10)	-39(19)
42(6)	11(19)	-31(11)	50(16)
51(6)	-13(20)	-8(11)	6(18)
40(5)	-30(18)	17(9)	7(16)
39(5)	67(23)	45(12)	-23(14)
59(11)	224(71)	194(38)	45(34)

Table 9

Final Parameters for Hydrogen Atoms for $C\ell Co(H_2dpg_2)(clan)$[a]

Atom [Bonded to]	Distance	x	y	z	B
H(B1)		303(9)	344(12)	153(8)	11.6(5.1)
H(B2)		352(7)	277(9)	439(5)	4.3(2.7)
H(2)[C(2)]	0.84(10)	514(7)	87(9)	325(5)	4.3(2.8)
H(3)[C(3)]	0.95(14)	627(9)	47(12)	260(7)	9.8(4.5)
H(5)[C(5)]	0.80(10)	445(6)	54(8)	93(5)	4.1(2.8)
H(6)[C(6)]	1.00(10)	336(7)	84(9)	152(5)	4.7(3.0)
H(7)[N(1)]	0.93(11)	305(7)	107(10)	264(6)	5.9(3.3)
H(8)[N(1)]	1.02(15)	382(9)	103(13)	332(8)	11.7(4.6)
H(1A)[C(1A)]	1.05(12)	558(7)	278(10)	135(6)	6.0(3.2)
H(2A)[C(2A)]	0.94(10)	680(6)	329(8)	89(5)	4.0(2.7)
H(3A)[C(3A)]	1.18(15)	759(9)	514(13)	117(7)	10.5(4.8)
H(4A)[C(4A)]	1.12(12)	711(7)	604(10)	227(6)	5.7(3.3)
H(5A)[C(5A)]	0.86(9)	601(6)	525(8)	227(5)	2.4(2.4)
H(1B)[C(1B)]	1.07(9)	654(6)	236(8)	320(5)	3.0(2.6)
H(2B)[C(2B)]	1.12(19)	796(11)	224(16)	398(9)	14.6(6.6)
H(3B)[C(3B)]	0.68(13)	792(9)	351(11)	487(7)	9.1(4.4)
H(4B)[C(4B)]	0.74(10)	690(7)	403(9)	533(6)	5.3(3.0)
H(5B)[C(5B)]	0.55(14)	586(9)	406(12)	471(7)	11.2(4.6)
H(1C)[C(1C)]	0.81(13)	76(8)	69(10)	352(7)	8.3(4.1)
H(2C)[C(2C)]	1.04(19)	3(12)	7(15)	403(9)	15.8(6.3)
H(3C)[C(3C)]	0.96(12)	-63(8)	140(10)	504(7)	8.2(4.0)
H(4C)[C(4C)]	0.92(12)	4(8)	305(10)	515(6)	6.0(3.0)
H(5C)[C(5C)]	1.00(8)	106(5)	362(6)	447(4)	0.5(1.9)
H(1D)[C(1D)]	1.05(9)	116(6)	175(7)	128(5)	3.0(2.4)
H(2D)[C(2D)]	1.10(9)	-41(6)	160(8)	52(5)	2.8(2.6)
H(3D)[C(3D)]	0.97(14)	-145(9)	219(12)	101(7)	10.1(4.4)
H(4D)[C(4D)]	1.04(10)	-136(6)	343(8)	212(5)	3.8(2.7)
H(5D)[C(5D)]	0.70(8)	25(5)	316(7)	224(4)	1.5(2.0)

[a]The hydrogen atom is given followed by the atom to which it is bonded in brackets, the corresponding bond distance (Å), the positional parameters with estimated standard deviations (x 10^{+3}), and the isotropic thermal parameters ($Å^2$).

The scattering factors for cobalt, oxygen, nitrogen, and carbon were from Hanson et al.,[29] those for hydrogen were from Stewart et al.,[30] and those for chlorine were from Doyle and Turner.[31] The observed and calculated structure factors are given in Table B-2. Lists of final positional and thermal parameters may be found in Tables 10 and 11.

Results and Discussion

The atomic numbering and thermal ellipsoids of $C\ell Co(H_2dmg)(dmg)(clan)$, $C\ell Co(H_2dpg_2)(clan)$, and $[Co(Hdmg)_2(clan)_2]C\ell$ are shown in ORTEP[54] drawings in Figures 1, 2, and 3, respectively. The individual bond distances for these three compounds together with those of two related compounds, $C\ell Co(H_2dmg)(dmg)(sulfa)$[46] and $[Co(Hdmg)_2(an)_2]C\ell$,[52] are tabulated in Table 12. The corresponding bond angles are given in Table 13.

In each case the two dmg or dpg groups are approximately planar as demonstrated by the deviations from least-squares planes in Tables 14-16. The dmg groups of each complex are linked by two intramolecular hydrogen bonds (see Table 17).

As in the case of $C\ell Co(H_2dmg)(dmg)(sulfa)$[46] the hydrogen bridges between the dmg groups in $C\ell Co(H_2dmg)(dmg)(clan)$ were found to be asymmetrical with both hydrogen atoms bonded to the same dmg ligand. The O(21)-H(B2) and O(22)-H(B1) distances of 1.13(8) and 1.16(8) Å, respectively, compared to the O(12)···H(B2) and O(11)···H(B1) distances of 1.36(8) and 1.37(8) Å indicate the formulation H_2dmg and dmg for the two

Table 10

The Final Atomic Parameters for Nonhydrogen Atoms of [$Co(Hdmg)_2(clan)_2$]$C\ell$.[a]

Atom	x	y	z	β_{11}	β_{22}
Co	0(0)	0(0)	0(0)	817(11)	628(5)
$C\ell$(1)	0(0)	50000(0)	0(0)	2653(30)	664(12)
$C\ell$(2)	32052(23)	26440(24)	55881(8)	5254(48)	6743(52)
O(11)	4450(2)	1508(2)	573(1)	97(4)	126(3)
O(12)	-3514(3)	531(2)	-1814(1)	125(5)	144(3)
N(1)	-846(3)	1678(2)	816(2)	116(5)	77(3)
N(11)	2490(3)	1399(2)	-160(2)	105(5)	83(3)
N(12)	-1339(3)	923(2)	-1288(1)	118(5)	91(3)
C(1)	97(4)	1928(3)	1978(2)	148(7)	90(3)
C(2)	2160(4)	2812(3)	2368(2)	195(8)	136(4)
C(3)	3103(5)	3034(4)	3474(3)	224(9)	231(6)
C(4)	1982(6)	2386(5)	4181(3)	317(11)	311(8)
C(5)	-77(6)	1504(5)	3818(3)	320(11)	300(8)
C(6)	-1012(4)	1282(4)	2704(2)	193(8)	185(5)
C(11)	2176(4)	2274(3)	-990(2)	159(7)	76(3)
C(12)	-124(4)	1982(3)	-1665(2)	185(7)	87(3)
C(13)	3887(4)	3459(3)	-1239(2)	216(8)	116(4)
C(14)	-937(5)	2830(4)	-2658(3)	289(10)	169(5)

[a]All values are x 10^4 except those for Co, $C\ell$(1) and $C\ell$(2) which are x 10^5. The estimated standard deviations are given in parentheses. The temperature factors are of the form: $\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}\ell^2 + \beta_{12}hk + \beta_{13}h\ell + \beta_{23}k\ell)]$.

Table 10 - extended

β_{33}	β_{12}	β_{13}	β_{23}
332(3)	226(12)	169(9)	-43(6)
873(8)	451(29)	1194(26)	131(15)
482(7)	-1987(79)	-431(28)	-982(29)
57(1)	9(5)	11(4)	-12(3)
57(1)	40(6)	-20(4)	15(3)
45(1)	28(6)	30(4)	-9(3)
47(1)	26(6)	30(4)	-21(3)
41(1)	53(6)	7(4)	-7(3)
47(2)	47(8)	27(5)	-24(4)
63(2)	-25(9)	59(6)	-42(5)
72(2)	-85(12)	-3(8)	-93(6)
49(2)	2(15)	-11(8)	-59(7)
51(2)	-22(15)	64(8)	1(7)
52(2)	-11(10)	36(6)	-12(5)
52(2)	42(7)	73(6)	-4(4)
46(2)	68(8)	56(6)	6(4)
77(2)	12(9)	109(7)	16(5)
68(2)	68(11)	47(8)	75(6)

Table 11

Final Parameters for Hydrogen Atoms for $[Co(Hdmg)_2(clan)_2]Cl^a$

Atom [Bonded to]	Distance	x	y	z	B
H(B1)[O(12)]	1.07(3)	-408(8)	-35(4)	-133(3)	5.5(0.8)
H(2)[C(2)]	0.85(3)	280(4)	321(3)	190(2)	3.5(0.6)
H(3)[C(3)]	0.91(4)	447(6)	361(4)	366(3)	6.0(0.8)
H(5)[C(5)]	0.98(4)	-92(6)	105(4)	431(3)	6.6(0.9)
H(6)[C(6)]	0.96(3)	-248(5)	73(3)	244(2)	3.9(0.6)
H(7)[N(1)]	0.88(2)	-299(4)	146(3)	64(2)	2.1(0.5)
H(8)[N(1)]	0.94(2)	-52(4)	262(3)	49(2)	2.7(0.5)
H(11)[C(13)]	0.90(4)	349(6)	440(4)	-131(3)	5.7(0.8)
H(12)[C(13)]	0.89(4)	417(7)	315(5)	-185(4)	9.0(1.2)
H(13)[C(13)]	0.91(4)	513(6)	353(5)	-67(3)	7.3(1.0)
H(14)[C(14)]	0.86(4)	-181(7)	217(5)	-314(3)	9.0(1.2)
H(15)[C(14)]	0.80(5)	-14(8)	360(6)	-274(4)	10.0(1.3)
H(16)[C(14)]	1.01(5)	-213(8)	337(6)	-252(4)	11.0(1.4)

[a]The hydrogen atom is given followed by the atom to which it is bonded in brackets, the corresponding bond distance (Å), the positional parameters with estimated standard deviations (x 10^{+3}), and the isotropic thermal parameters (Å^2).

Figure 1

An ORTEP drawing of $C\ell Co(H_2dmg)(dmg)(clan)\cdot 2H_2O$ showing the atomic numbering and thermal ellipsoids. The hydrogen atoms and water molecules have been omitted for clarity.

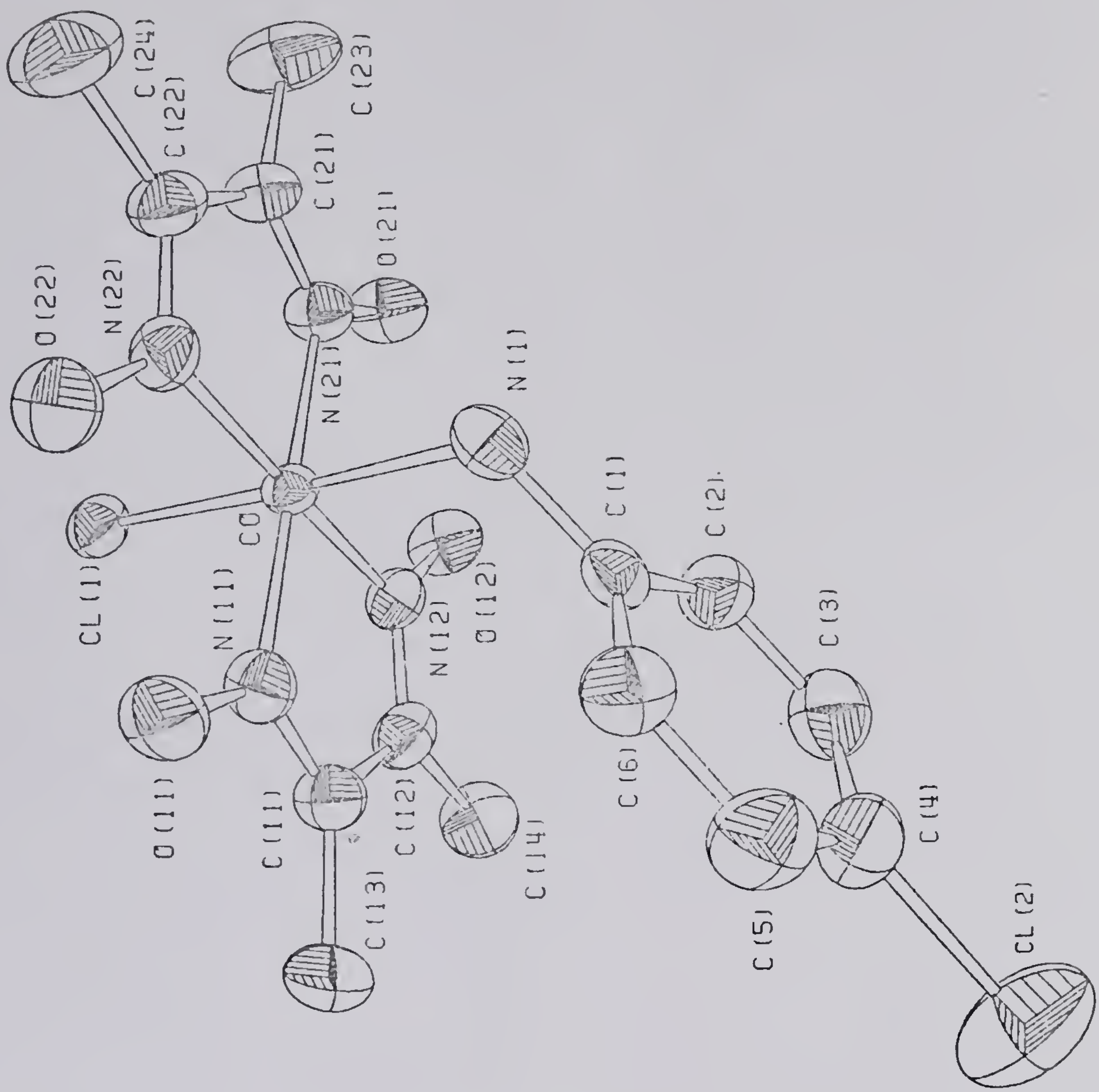
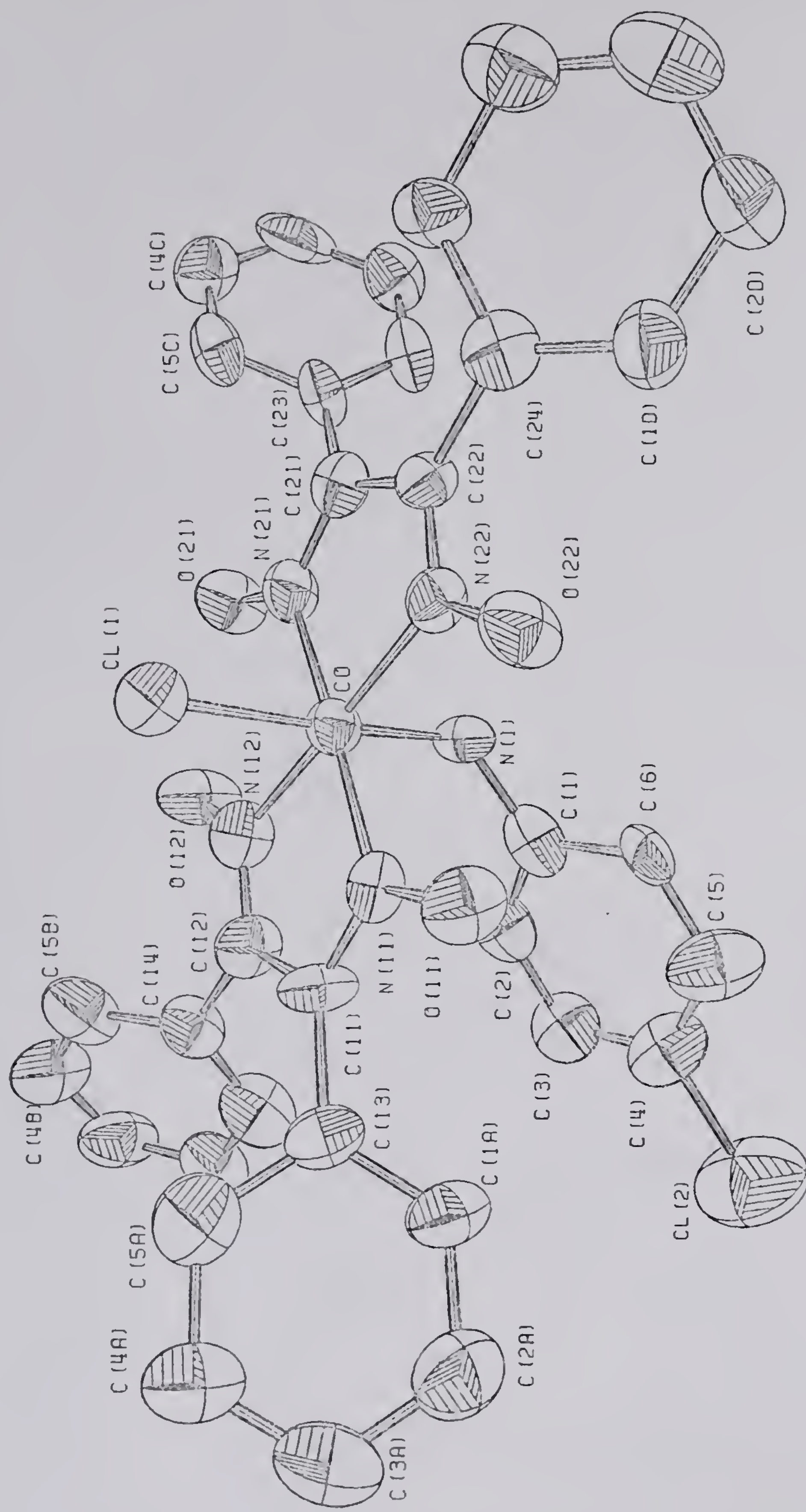

C (24)
C (22)
C (23)
C (21)
O (21)
O (22)
N (22)
N (21)
N (1)
CO
CL (1)
C (1)
C (2)
N (11)
N (12)
O (12)
C (3)
O (11)
C (11)
C (12)
C (6)
C (4)
C (14)
C (13)
C (5)
CL (2)

Figure 2

An ORTEP drawing of $C\ell Co(H_2dpg_2)(clan) \cdot C_2H_5OH$ showing the atomic numbering and thermal ellipsoids. The hydrogen atoms and C_2H_5OH molecule have been omitted.



C (4C)
C (5C)
C (23)
C (21)
N (21)
O (21)
CL (1)
CO
N (12)
N (1)
N (22)
O (22)
C (22)
C (24)
C (1D)
C (2D)
O (12)
C (12)
C (5B)
C (14)
C (4B)
C (11)
N (11)
O (11)
C (2)
C (1)
C (6)
C (5)
C (3)
C (4)
C (13)
C (1A)
CL (2)
C (5A)
C (4A)
C (2A)
C (3A)

Figure 3

An ORTEP drawing of $[Co(Hdmg)_2(clan)_2]C\ell$ showing the atomic numbering and thermal ellipsoids. The hydrogen atoms have been omitted.

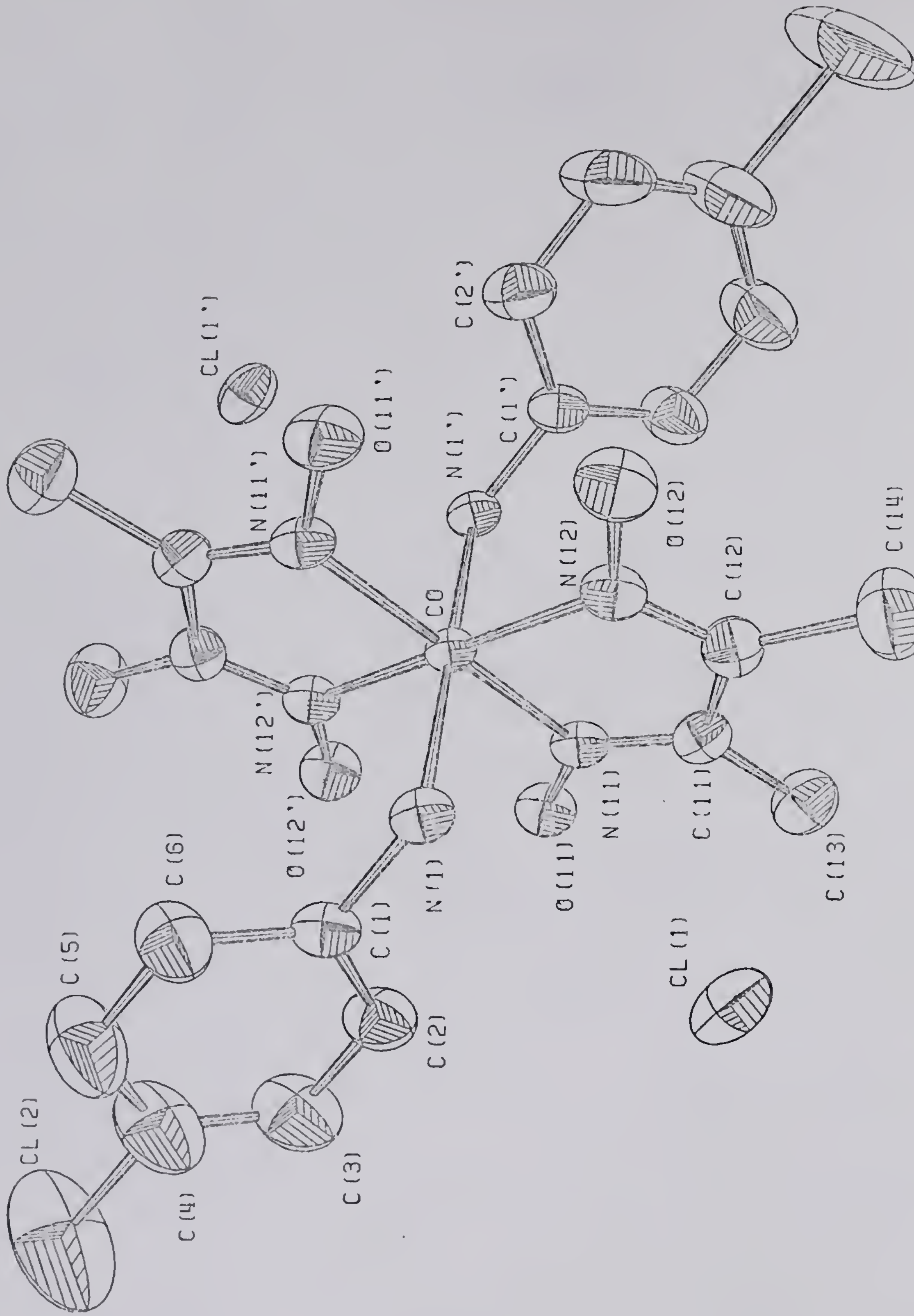

CL (1')
C (2')
Ø (11')
N (1')
C (1')
N (11')
Ø (12)
N (12)
C (12)
C (14)
CO
N (12')
Ø (12')
C (6)
N (1)
Ø (11)
N (11)
C (11)
C (13)
C (5)
C (1)
CL (1)
C (2)
CL (2)
C (3)
C (4)

Table 12
Selected Interatomic Distances (Å) in Some Cobaloxime Complexes with Their Estimated Standard Deviations.[a]

	$C\ell Co(H_2dmg)(clan)$	$C\ell Co(H_2dpg)_2(clan)$
Co-N(1)	1.999(6)	1.946(11)
Co-N(11)	1.872(5)	1.908(9)
Co-N(12)	1.884(5)	1.935(11)
N(11)-O(11)	1.337(6)	1.356(11)
N(12)-O(12)	1.329(6)	1.316(12)
N(11)-C(11)	1.311(8)	1.298(15)
N(12)-C(12)	1.308(8)	1.292(16)
C(11)-C(12)	1.457(9)	1.455(16)
C(11)-C(13)	1.488(10)	1.487(17)
C(12)-C(14)	1.487(10)	1.536(18)
O(11)···O(22)	2.497(7)	2.540(11)
O(11)-H(B)	1.37(8)	1.41(14)
O(12)-H(B)	1.36(8)	1.30(10)
Co-Cℓ(1)	2.257(2)	2.244(4)
Co-N(21)	1.908(5)	1.887(10)
Co-N(22)	1.906(5)	1.897(9)
N(21)-O(21)	1.348(6)	1.321(12)
N(22)-O(22)	1.359(6)	1.337(11)
N(21)-C(21)	1.280(8)	1.331(16)
N(22)-C(22)	1.288(8)	1.313(14)
C(21)-C(22)	1.468(9)	1.483(15)
C(21)-C(23)	1.486(11)	1.457(17)
C(22)-C(24)	1.498(11)	1.464(17)
O(12)···O(21)	2.479(7)	2.460(12)
O(21)-H(8)	1.13(8)	1.16(10)
O(22)-H(B)	1.16(8)	1.17(15)

*Distance given is for O(11)···O(12')≡O(12)···O(11')

[a]Values for $[Co(H_2dmg_2)(an)_2]C\ell$ are listed with atomic numbering corresponding to the compounds of this work.

Table 12 - extended

$C\ell Co(H_2dmg_2)(sulfa)$[46]	$[Co(H_2dmg_2)(clan)_2]C\ell$	$[Co(H_2dmg_2)(an)_2]C\ell$[52]
2.023(8)	2.003(2)	2.001(5)
1.870(8)	1.906(2)	1.885(6)
1.884(8)	1.889(2)	1.889(5)
1.323(11)	1.340(3)	1.353(6)
1.344(11)	1.362(3)	1.333(6)
1.289(14)	1.299(3)	1.286(10)
1.293(13)	1.290(3)	1.303(10)
1.494(16)	1.477(4)	1.463(7)
1.532(17)	1.483(4)	1.482(12)
1.488(16)	1.485(4)	1.476(11)
2.507(11)	2.495(3)*	2.491(8)*
1.50	1.44(3)	1.29
1.60	1.07(3)	1.21
2.235(3)		
1.905(8)		
1.896(8)		
1.326(10)		
1.338(11)		
1.292(12)		
1.290(14)		
1.447(17)		
1.494(17)		
1.488(16)		
2.479(11)		
0.90		
1.04		

Table 13
Selected Intramolecular Angles (°) in Some Cobaloxime Complexes with Their Estimated Standard Deviations.[a]

	$C\ell Co(H_2dmg_2)(clan)$	$C\ell Co(h_2dpg_2)(clan)$
N(1)-Co-N(11)	90.5(2)	94.8(4)
N(1)-Co-N(12)	91.5(2)	92.1(4)
N(1)-Co-N(21)	88.4(2)	87.1(4)
N(1)-Co-N(22)	88.6(2)	88.6(4)
N(11)-Co-N(12)	82.6(2)	81.3(4)
N(11)-Co-N(22)	98.8(2)	100.0(4)
N(11)-Co-N(21)	178.8(2)	177.5(4)
N(12)-Co-N(21)	98.1(2)	97.0(4)
N(12)-Co-N(22)	178.6(2)	178.5(4)
N(21)-Co-N(22)	80.6(2)	81.7(4)
Cℓ(1)-Co-N(11)	90.6(2)	87.7(3)
Cℓ(1)-Co-N(12)	90.6(2)	89.1(3)
Cℓ(1)-Co-N(21)	90.5(2)	90.4(3)
Cℓ(1)-Co-N(22)	89.4(2)	90.2(3)
Cℓ(1)-Co-N(1)	177.8(2)	177.4(3)
Co-N(1)-C(1)	119.7(4)	118.6(8)
Co-N(11)-O(11)	121.9(4)	123.3(7)
Co-N(12)-O(12)	122.2(4)	121.2(8)
Co-N(21)-O(21)	123.2(4)	123.5(8)
Co-N(22)-O(22)	123.3(4)	120.7(7)
Co-N(11)-C(11)	116.0(4)	116.7(8)
Co-N(12)-C(12)	115.6(4)	114.1(9)
Co-N(21)-C(21)	116.6(4)	116.8(8)
Co-N(22)-C(22)	117.0(4)	117.4(8)
O(11)-N(11)-C(11)	122.1(5)	119.7(9)
O(12)-N(12)-C(12)	122.3(5)	123.8(11)
O(21)-N(21)-C(21)	120.3(5)	119.4(10)
O(22)-N(22)-C(22)	119.8(5)	121.7(10)
N(11)-O(11)···O(22)	99.7(3)	95.9(6)
N(12)-O(12)···O(21)	99.7(3)	99.2(7)
N(21)-O(21)···O(12)	96.9(3)	98.2(7)
N(22)-O(22)···O(11)	96.0(3)	100.1(6)

Table 13 - extended

$C\ell Co(H_2dmg_2)(sulfa)$[46]	$[Co(H_2dmg_2)(clan)_2]C\ell$	$[Co(H_2dmg_2)(an)_2]C\ell$[52]
90.5(3)	89.8(1)	91.5(4)
91.7(3)	93.2(1)	93.0(5)
89.3(3)		
87.8(3)		
82.0(4)	80.8(1)	80.8(3)
98.7(4)		
179.3(4)		
98.7(3)		
179.2(4)		
80.6(3)		
89.6(3)		
88.5(3)		
90.5(3)		
91.9(3)		
179.7(2)		
119.1(6)	119.7(1)	119.5(7)
123.0(6)	121.3(1)	121.4(6)
122.6(6)	122.7(1)	122.9(7)
121.6(6)		
123.6(6)		
116.4(7)	116.9(2)	116.8(9)
117.4(7)	117.7(2)	117.8(9)
116.3(7)		
116.8(7)		
120.5(9)	121.8(2)	121.8(12)
120.0(8)	119.6(2)	119.2(10)
122.2(8)		
120.1(9)		
98.3(6)		
97.8(6)		
99.2(5)		
96.8(6)		

Table 13 - continued

	$C\ell Co(H_2dmg_2)(clan)$	$C\ell Co(H_2dpg_2)(clan)$
N(11)-C(11)-C(12)	112.8(6)	112.1(10)
N(11)-C(11)-C(13)	122.9(6)	125.6(11)
N(12)-C(12)-C(11)	113.1(6)	115.5(11)
N(12)-C(12)-C(14)	122.5(6)	119.5(11)
N(21)-C(21)-C(22)	113.5(6)	112.2(10)
N(21)-C(21)-C(23)	112.4(7)	120.9(11)
N(22)-C(22)-C(21)	112.3(6)	111.9(10)
N(22)-C(22)-C(24)	123.2(6)	126.0(11)
C(13)-C(11)-C(12)	124.2(6)	122.3(11)
C(14)-C(12)-C(11)	124.4(6)	125.0(11)
C(23)-C(21)-C(22)	124.1(6)	126.8(11)
C(24)-C(22)-C(21)	124.4(6)	122.2(10)

[a]The atomic numbering of $Co(H_2dmg_2)(an)_2C\ell$[52] has been changed to correspond to that of compounds of this work.

Table 13 - continued - extended

$ClCo(H_2dmg_2)(sulfa)$[46]	$[Co(H_2dmg_2)(clan)_2]Cl$	$[Co(H_2dmg_2)(an)_2]Cl$[52]
113.3(9)	112.2(2)	112.4(10)
125.0(10)	125.0(2)	124.6(16)
110.7(9)	112.5(2)	112.2(9)
124.0(10)	124.1(2)	125.0(16)
113.1(9)		
120.7(10)		
113.1(9)		
122.9(10)		
121.7(10)	122.9(2)	123.0(12)
125.3(10)	123.4(2)	122.9(13)
126.1(10)		
123.6(10)		

ligands. This is in contrast to results reported for various $Co(H_2dmg_2)$ complexes[40,47,48,50,52] as well as for $Fe(H_2dmg_2)$-(imidazole)$_2$,[55] $Ni(H_2dmg_2)$,[56] and $Cu(H_2dmg_2)$,[57] where either the hydrogen bridges were assumed to be equidistant from the two oxygen atoms or the ligands were monoprotonated. The assumption of a symmetrical bridge may have in part been based on the earlier IR spectroscopic work on $M(H_2dmg_2)$ complexes where the weak band due to an O-H vibration near 1725 cm^{-1} was assumed to indicate a very short and symmetrical O-H-O bridge.[19,20] McFadden and McPhail[51] reported the structure of $Co(H_2dmg_2)(CH_3)(H_2O)$ in which both bridging hydrogen atoms if ordered are required crystallographically to be on one dmg ligand. No comment was made concerning the bridging hydrogen atoms.

Although both hydrogen bridges in $C\ell Co(H_2dpg_2)$(clan) appear to be shifted toward one dmg where the O(21)-H(B2) and O(22)-H(B1) distances are 1.16(10) and 1.17(15) Å while the O(12)-H(B2) and O(11)-H(B1) distances are 1.30(10) and 1.41 (14) Å, the experimental uncertainty is too large to show that result to be significant.

The hydrogen bridges in $[Co(Hdmg)_2(clan)_2]C\ell$ are not symmetrical and each dmg is singly protonated. The O(12)-H(B1) distance is 1.07(3) Å and the O(11)···H(B1) distance is 1.44 (3) Å. The gross structure is very similar to that of $[Co(Hdmg)_2(an)_2]C\ell$.

Bowman et al.[55] suggested the N-O distance to be a sensitive indicator of the position of the bridging hydrogen.

Table 14

Deviations and Equations of Selected Least-Squares Planes in $C\ell Co(H_2dmg)(dmg)(clan)$[a]

(a) Deviations (Å x 10^{+3})

	Plane 1	Plane 2	Plane 3	Plane 4
Co	5	-1796	0*	72
O(11)	25		-2574	209
O(12)	-23		2533	80
N(11)	-2*		-1260	175
N(12)	2*		1218	140
C(11)	4*		-775	251
C(12)	-4*		682	220
C(13)	73		-1633	413
C(14)	41		1498	330
O(21)	34		2602	-22
O(22)	-79		-2548	-55
N(21)	48		1269	1*
N(22)	7		-1197	-1*
C(21)	113		795	-2*
C(22)	94		-673	2*
C(23)	230		1664	24
C(24)	143		-1482	-17
N(1)	2004	-41	0*	
C(1)	2752	-12*	0*	
C(2)	3092	5*	1197	
C(3)	3767	5*	1204	
C(4)	4105	-9*	18	
C(5)	3790	3*	-1193	
C(6)	3112	8*	-1204	
Cℓ(2)	4946	-28	5	
Cℓ(1)	-2252		-29	

(b) Coefficients of the Plane Equation[58]

$Ax + By + Cz = D$

Plane	A	B	C	D
1	0.8529	0.4975	0.1583	1.6954

Table 14 - continued

Plane	A	B	C	D
2	0.9995	0.0282	0.0142	1.6347
3	0.0208	-0.3098	0.9506	1.7440
4	0.8174	0.5536	0.1594	1.8108

[a]The deviations of atoms used to define the plane are marked with an asterisk.

Table 15

Deviations and Equations of Selected Least-Squares Planes in $C\ell Co(H_2dpg_2)(clan)$[a]

(a) Deviations (Å x 10^{+3})

	Plane 1	Plane 2	Plane 3	Plane 4
Co	19	-1932	0*	29
O(11)	-56		1350	-101
O(12)	122		-2807	192
N(11)	17*		160	2
N(12)	-18*		-1881	24
C(11)	-30*		-945	-30
C(12)	30*		-2118	62
C(13)	-179		-1048	-195
C(14)	94		-3571	149
O(21)	-5			60
O(22)	-37			-87
N(21)	-43			-8*
N(22)	28			8*
C(21)	-9			13*
C(22)	-1			-13*
C(23)	93			133
C(24)	-58			-89
N(1)	1958	-148	0*	
C(1)	2755	-18*	0*	
C(2)	3166	4*	-1171	
C(3)	3843	16*	-1184	
C(4)	4069	-20*	10	
C(5)	3720	5*	1166	
C(6)	3076	14*	1205	
Cℓ(2)	4901	-1	-10	
Cℓ(1)	-2223		24	
C(1A)	676			
C(2A)	510			
C(3A)	-529			
C(4A)	-1417			
C(5A)	-1255			

Table 15 - continued

	Plane 1	Plane 2	Plane 3	Plane 4
C(1B)	1094			
C(2B)	1237			
C(3B)	427			
C(4B)	-641			
C(5B)	-821			
C(1C)				1232
C(2C)				1380
C(3C)				361
C(4C)				-734
C(5C)				-827
C(1D)				571
C(2D)				554
C(3D)				-230
C(4D)				-874
C(5D)				-858

(b) Coefficients of the Plane Equation[58]
$Ax + BY + Cz = D$

Plane	A	B	C	D
1	0.1954	-0.9752	-0.1036	3.3476
2	-0.2301	-0.9634	0.1374	1.9549
3	0.5744	0.0297	0.8181	-7.1571
4	0.1976	-0.9769	-0.0813	3.2302

[a]The deviations of atoms used to define the plane are marked with an asterisk.

Table 16
Deviations and Equations of Selected Least Squares Planes in $[Co(Hdmg)_2(clan)_2]C\ell$[a]

(a) Deviations (Å x 10^{+3})

	Plane 1	Plane 2	Plane 3
Co	10	-1772	0*
O(11)	36		2519
O(12)	14		-523
N(11)	0*		1902
N(12)	0*		428
C(11)	1*		2567
C(12)	-1*		1677
C(13)	26		4046
C(14)	11		2173
N(1)	2009	-28	0*
C(1)	2799	-2*	0*
C(2)	3030	2*	1194
C(3)	3758	-1*	1208
C(4)	4257	0*	37
C(5)	4048	0*	-1168
C(6)	3312	1*	-1174
Cℓ(2)	5159	-33	53

(b) Coefficients of the Plane Equation[59]
$Ax + By + Cz = D$

Plane	A	B	C	D
1	-0.4938	0.6723	0.5515	-0.0101
2	-0.5672	0.8236	0.0096	1.7716
3	0.7336	0.6606	-0.1594	0.0000

[a]The deviations of atoms used to define the plane are marked with an asterisk.

Table 17

Hydrogen Bonds with Estimated Standard Deviations Given in Parentheses.

Bond	Position of	Distances (Å)			Angles (°)
D-H···A[a]	A	D-H	H···A	D···A	D-H···A
$C\ell Co(H_2dmg_2)(clan)$					
O(21)-H(B2)···O(12)	x,y,z	1.13(8)	1.36(8)	2.479(7)	166(7)
O(22)-H(B1)···O(11)	x,y,z	1.16(8)	1.37(8)	2.497(7)	161(6)
N(1)-H(7)···O(w1)	x,y,z	1.03(7)	1.92(7)	2.900(7)	157(6)
N(1)-H(8)···O(w2)	x,y,z	0.83(6)	2.04(7)	2.849(7)	164(6)
O(w1)-H(w1)···Cℓ(1)	1+x,y,z	0.70(8)	2.76(8)	3.284(6)	134(8)
O(w1)-H(w1')···O(11)	1-x,1-y,-z	0.80(13)	2.34(12)	2.823(7)	120(11)
O(w2)-H(w2)···O(12)	1-x,1-y,1-z	0.79(7)	2.05(7)	2.813(6)	164(8)
O(w2)-H(w2')···Cℓ(1)	1+x,y,z	0.71(7)	2.56(7)	3.226(5)	157(7)
$[Co(H_2dmg_2)(clan_2]C\ell$					
O(12)-H(B1)···O(11)	-x,-y,-z	1.07(3)	1.44(3)	2.495(3)	170(3)
N(1)-H(7)···O(11)	-1+x,y,z	0.88(2)	2.07(3)	2.918(3)	163(2)
N(1)-H(8)···Cℓ(1)	x,y,z	0.94(2)	2.17(2)	3.100(2)	168(2)
$C\ell Co(H_2dpg_2)(clan)$					
O(21)-H(B1)···O(12)	x,y,z	1.16(10)	1.30(10)	2.460(12)	172(10)
O(22)-H(B2)···O(11)	x,y,z	1.17(15)	1.41(14)	2.540(11)	159(13)
O(S1)···· O(22)	x,y,z			2.852(15)	

[a]Donor-Hydrogen···Acceptor, D-H at x,y,z.

Dissimilar N-O bond lengths should indicate the hydrogen is not symmetrically located and is closer to the dmg with the longer bond. This holds true in $C\ell Co(H_2dmg)(dmg)(clan)$ where the N-O distances appear to be different. The N(21)-O(21) and N(22)-O(22) distances of 1.348(6) and 1.359(6) Å in the diprotonated dmg are longer than the N(12)-O(12) and N(11)-O(11) distances of 1.329(6) and 1.337(6) Å in the dianionic dmg. Using the significance test described by Cruickshank and Robertson[60] the N(21)-O(21) distance is possibly longer than the N(12)-O(12) with a t_o value of 2.24 and the N(22)-O(22) bond is significantly longer than the N(11)-O(11) bond with a t_o value of 2.59. Also, in $[Co(Hdmg)_2(clan)_2]C\ell$ the N(12)-O(12) bond of 1.362(3) Å is significantly longer than the N(11)-O(11) bond of 1.340(3) Å, where the bridging hydrogen atom is bonded to O(12). Neither the N-O distances nor the bridging O-H distances in $C\ell Co(H_2dpg_2)(clan)$ are significantly different. In $[Co(Hdmg)_2(an)_2]C\ell$ where the hydrogen atoms are not significantly removed from a symmetrical position, the N(12)-O(12) distance is shorter than that of N(11)-O(11). The difference in these two bond lengths of 1.333(6) and 1.353(6) Å is of possible significance (t_o = 2.36). The sensitivity of the N-O bond as an indicator of the bridge position is questionable. The N-O bonds are not significantly different in $C\ell Co(H_2dmg)(dmg)(sulfa)$ when both bridging hydrogen atoms are shifted to one dmg. In the closely related dimethyl(3,3'-trimethylenedinitrilo)bis-(butan-2-one-oximato)cobalt(III) complex the two N-O distances are equal

even though an asymmetric hydrogen bridge is clearly indicated by the difference Fourier syntheses.[61] Although a difference in the N-O bond lengths as a function of protonation is reasonable, there are very few structures so precisely determined that this comparison can be made. Hence, no general conclusion may be made. However, when a significant difference in the N-O distances has been found and the bridging hydrogen atom has been precisely located, the hydrogen atom is associated with the longer N-O bond.

Another point in support of the formulation $C\ell Co(H_2dmg)$-(dmg)(clan) is the difference in the Co-N bond lengths. The Co-N distances on the H_2dmg side are 1.908(5) and 1.906(5) Å compared to distances of 1.872(5) and 1.884(5) Å on the dmg side. The differences in the Co-N bond lengths are significant and the shorter distances involve the dianionic group. This holds true in the other cases where the presence of both H_2dmg and dmg ligands has been indicated. In $C\ell Co(H_2dmg)$(dmg)-(sulfa)[46] and in $Co(H_2dmg_2)(CH_3)(H_2O)$[51] the distances from the cobalt atom to the dianionic ligand are shorter than the distances to the neutral H_2dmg ligand. This is not the case in $C\ell Co(H_2dpg_2)$(clan) where the distances from the cobalt atom to what would be the dpg dianionic ligand, 1.935(11) and 1.908 (9) Å, appear to be longer than the corresponding distances to the H_2dpg ligand, 1.887(10) and 1.897(9) Å. These differences together with the apparent positions of the bridging hydrogen atoms (vide supra) in $C\ell Co(H_2dpg_2)$(clan) are of questionable significance.

For the mononegative ligands in $[Co(Hdmg)_2(clan)_2]C\ell$ the Co–N distances are significantly different. However, N(12) which is bonded to the protonated oxygen atom is closer to the cobalt atom than is N(11) with distances of 1.889(2) and 1.906 (2) Å, respectively. The same relationship holds in $Fe(Hdmg)_2$-$(imidazole)_2$,[55] the only other $M(Hdmg)_2$ complex whose X-ray structure precisely places one bridging hydrogen on each dmg and shows a significant difference in the metal to nitrogen distance.

An unsymmetrical hydrogen-bonding system involving two similar atoms may be fluxional.[62] In such a system two equilibrium positions, i.e. potential wells, exist for the hydrogen atom. Each of these positions may be considered as having the hydrogen atom covalently bonded to one atom and hydrogen bonded to the other. For the system to be truly fluxional the energy barrier between the two positions must be thermally accessible. Depending on the relative depths of the potential wells, the energy barrier between them, and the thermal energy of the system the position of the hydrogen atom as indicated by X-ray diffraction experiments would vary. Because of the diffuse appearance of the bridging hydrogen atoms of the $M(H_2dmg_2)$ complexes in difference Fourier syntheses, a fluxional system with two potential wells of unequal depth seems reasonable. The relative populations of the two positions will depend somewhat on the depths of the potential wells. The experimentally determined position (or positions) of the hydrogen atom will reflect these populations. As the depths of the

potential wells approach equivalence and as the energy barrier between them becomes smaller the position of the hydrogen atom will become experimentally more uncertain. A fluxional system could, in part, account for the difficulty in precisely locating the bridging hydrogen atoms in $M(H_2dmg_2)$ complexes.

The orientation of the 4-chloroaniline ligand in the complexes of this study is quite intriguing. A projected view down the Co-N(1) bond for $C\ell Co(H_2dmg)(dmg)(clan)$ is shown in Figure 4. A similar view for $[Co(Hdmg)_2(clan)_2]C\ell$ is given in Figure 5(a) and one for $C\ell Co(H_2dpg_2)(clan)$ is given in Figure 5(b). In $C\ell Co(H_2dmg)(dmg)(clan)$, as in $C\ell Co(H_2dmg)(dmg)(sulfa)$[46] the aromatic ring of the aniline is oriented over the dianionic dmg ligand. The orientation angle, i.e. the dihedral angle between the planes having Co-N(1) in common with one containing C(1) and the other containing the bisector of the angle N(11)-Co-N(12), for $C\ell Co(H_2dmg)(dmg)(clan)$ is 0.9° and for $C\ell Co(H_2dmg)(dmg)(sulfa)$ is 1.8° as given in Table 18. In $[Co(Hdmg)_2(clan)_2]C\ell$ and in $[Co(Hdmg)_2(an)_2]C\ell$ the benzene rings are skewed relative to the equatorial ligands with orientation angles of 53.9° and 58.3°, respectively. It seems significant that in the former pair of $Co(H_2dmg)(dmg)$ type complexes the rings align while in the latter pair of $Co(Hdmg)_2$ type complexes the rings are skewed. Although the benzene ring of the aniline is tipped from being parallel to the dmg plane by ca. 30° as in other similar complexes (see Table 18) the alignment and the distances between the two planes in $C\ell Co(H_2dmg)(dmg)(clan)$ suggest a π-type interaction. The

Figure 4

A projected view along Co-N(1) for $C\ell Co(H_2dmg)(dmg)(clan)$.

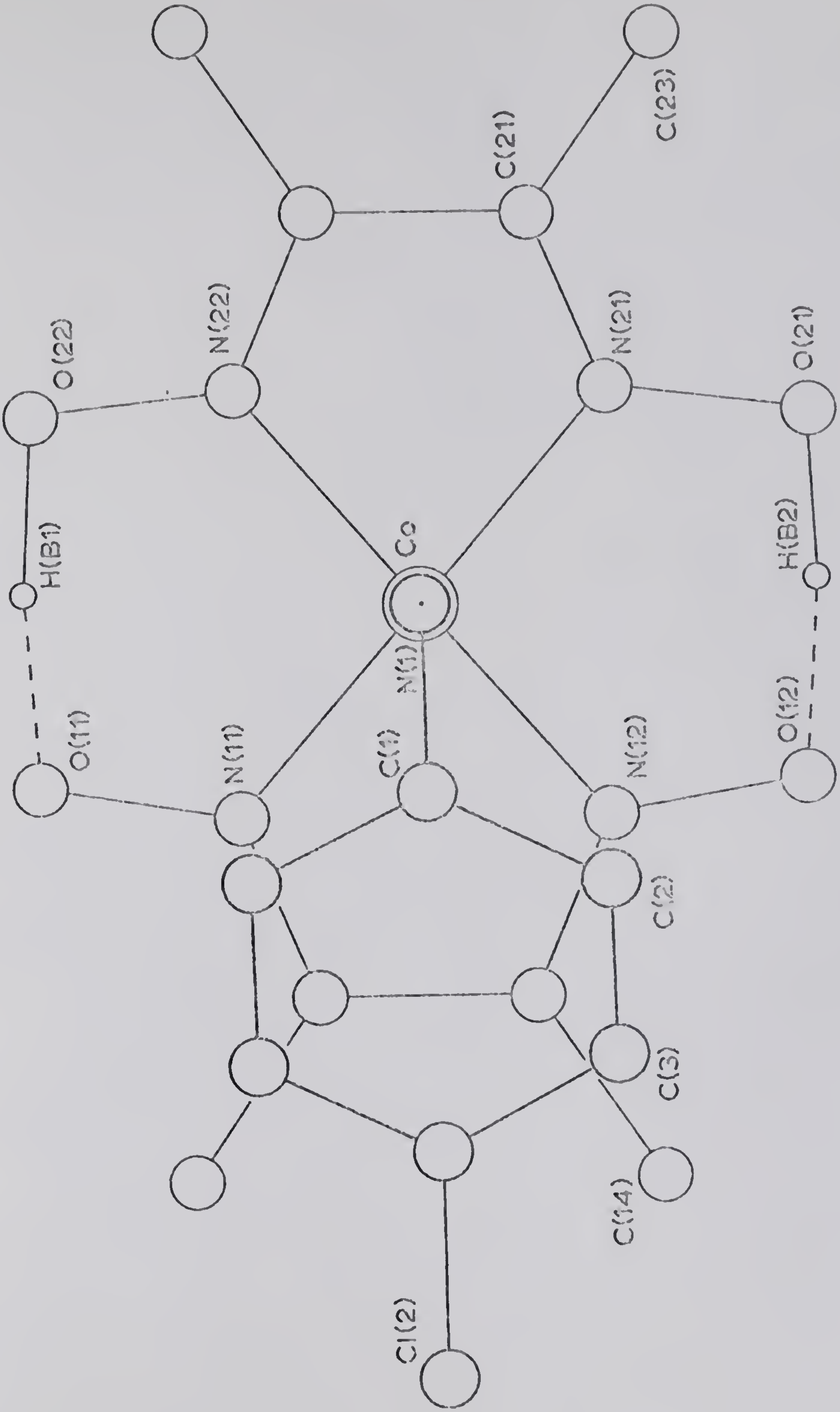
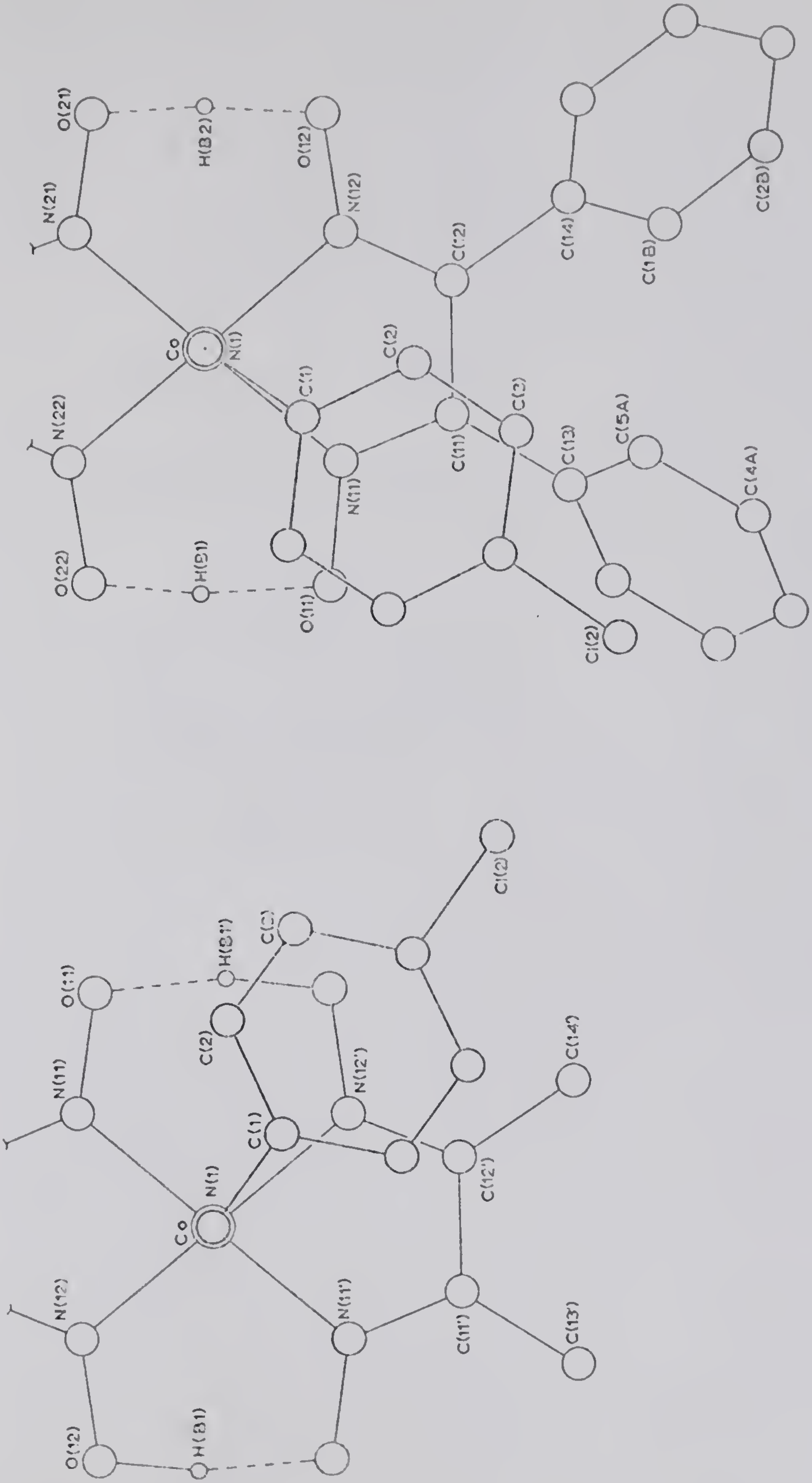

C(23)
C(21)
O(22)
N(22)
N(21)
O(21)
H(B1)
Co
H(B2)
N(1)
O(11)
N(11)
C(1)
N(12)
O(12)
C(2)
C(3)
C(14)
Cl(2)

Figure 5

A projected view along Co-N(1) for (a) $[Co(Hdmg)_2(clan)_2]C\ell$ and (b) $C\ell Co(H_2dpg_2)(clan)$.


O(21)
H(B2)
O(12)
N(21)
N(12)
Co
N(1)
C(12)
C(14)
C(1B)
C(2B)
C(2)
C(1)
N(22)
C(11)
C(3)
C(13)
C(5A)
C(4A)
N(11)
O(22)
H(B1)
O(11)
Cl(2)
O(11)
H(B1')
C(2)
N(11)
C(1)
N(12')
C(14')
N(1)
C(12')
N(12)
N(11')
C(11')
C(13')
O(12)
H(B1)
Cl(2)

(b)

(a)

Table 18

Dihedral Angles Formed by Selected Planes[a] in Some Cobaloxime Complexes

Intersecting Planes	Angles (°)		
	$C\ell Co(H_2dmg_2)$(clan)	$C\ell Co(H_2dpg_2)$(clan)	$C\ell Co(H_2dmg_2)$(sulfa)[46]
1-2	29.7	28.3	25.2
1-3	89.2	89.9	88.9
1-4	3.8	1.3	5.6
2-3	88.5	87.2	88.5
2-4	33.4	27.8	30.8
3-4	89.8	89.0	89.2
3-5	0.9	36.4	1.8

[a]Planes 1 to 4 are least-squares planes as defined in Tables 14-16 . Plane 1 is defined by N(11), N(12), C(11), and C(12). Plane 2 is defined by the carbon atoms in the benzene ring of the aniline ligand. Plane 3 is defined by Co, N(1), and C(1). Plane 4 is defined by N(21), N(22), C(21), and C(22). Plane 5 contains Co, N(1), and the bisector of the angle N(11)-Co-N(12).

Table 18 - extended

Intersecting Planes	Angles (°)	
	[Co(H_2dmg$_2$)(clan)$_2$]Cℓ	[Co(H_2dmg$_2$)(an)$_2$]Cℓ[52]
1-2	33.0	32.9
1-3	89.7	86.9
1-4	(180)	(180)
2-3	82.7	86.9
2-4		
3-4		
3-5	53.8	58.3

distances from the dmg plane to C(1), C(2), and C(6) given in Table 14 are substantially less then the 3.40 Å interplanar distance in graphite.[63] A proton transfer occurring from one Hdmg ligand to the other would increase the electron density within the π-system of the formed dianion. An interaction by which the filled π orbitals of the dmg overlap with the empty π^* orbitals of the aniline would enhance the basicity of the aniline ligand. The complex formed would be stronger than might be expected based on the K_b value alone. This same argument applies to $C\ell Co(H_2dmg)(dmg)(sulfa)$[46] which was the first example of ligand-induced proton shift in a molecular complex. While the positions of the bridging protons in $C\ell Co(H_2dmg)(dmg)(clan)$ and $[Co(Hdmg)_2(clan)_2]C\ell$ are well defined, the bridge in $C\ell Co(H_2dpg_2)(clan)$ is ill defined and the orientation angle of 36.7° is an intermediate value (see Table 18). The O···O distances in this complex show more variation than those in other related complexes as shown in Table 12. The 0.08 Å difference in the O...O distances is the same as for the corresponding N···N distances. The N(12)···N(21) separation is 2.836(15) Å and the N(11)···N(22) distance is 2.914(13) Å. Concurring with these observed distancces, the N(12)-Co-N(21) angle of 97.0(4)° is more acute than the N(11)-Co-N(22) angle of 100.0(4)°. None of the other compounds examined shows any significant differences in the corresponding distances and angles between the diglyoxime ligands.

A comparison of mean bonding distances for each of the reported $Co(H_2dmg_2)$ complexes may be made from Table 19. There appears to be little variation in the average Co-N distances or in the average dimensions within the equatorial dimethylglyoxime ligands as a function of the axial ligand.

Those complexes having chloride as an axial ligand show a definite variation with the nature of the trans ligand. The longest Co-Cℓ distance is found where tpp is the trans ligand. This is not surprising since phosphines are known to have a very large trans-influence[64] but the small influence the tpp ligand exerts on the trans-chlorine atom compared to that of an ammonia ligand is unexpected.[40] There is no significant difference in the Co-N(1) distance involving a clan ligand whether it is trans to a chlorine atom or trans to another clan ligand. The trans-influence appears to occur in $Co(H_2dmg_2)$ complexes but not to a large extent.

The Co-Y distances in the $XCo(H_2dmg_2)Y$ complexes where Y is a ligand with an sp^3 nitrogen, increase in the following order of Y: NH_3 < an $\sim$ clan < sulfa (see Table 19). This series can be rationalized in terms of the relative K_b's for sulfa (2.3×10^{-12}),[65] clan (9.6×10^{-11}),[66] aniline (4.0×10^{-10}),[66] and ammonia (1.8×10^{-5}).[67] Brückner and Randaccio[40] did not consider the K_b's of the different nitrogen donors in their argument of the trend in trans-influencing ligands, X, upon the Co-N bond. The same Co-N distances were used for NH_3 and aniline complexes in their argument for basing the extent of trans-influence on the σ-donor power of the trans

Table 19

A Summary of the Average Bond Distances (Å) in $XYCo(H_2dmg_2)$ Complexes.[a,b,c,d]

X	Y	Co-X	Co-Y	Co-N	N-O
clan	Cℓ	1.999(6)	2.257(2)	1.893(5)	1.343(6)
clan	clan	2.003(2)		1.898(2)	1.351(3)
*clan	Cℓ	1.946(11)	2.244(4)	1.907(11)	1.333(12)
sulfa	Cℓ	2.023(8)	2.235(3)	1.889(8)	1.333(11)
NH_3	Cℓ	1.965(4)	2.251(1)	1.890(5)	1.346(10)
tpp	Cℓ	2.327(4)	2.277(4)	1.89 (1)	1.343(9)
$SbPh_3$	Cℓ	2.54 (2)	2.25 (2)	1.95 (2)	
an	an	2.001(5)		1.887(6)	1.343(6)
CH_3	H_2O	1.990(5)	2.058(3)	1.890(3)	1.352(5)
C-py	P(n-But)$_3$	1.979(1)	2.339(1)	1.876(3)	1.339(7)
CH_2COOCH_3	py	2.04	2.04	1.88	1.37
DDT	py	1.97 (1)	2.04 (1)	1.88 (1)	1.35 (2)

[a]The ligands X and Y are approximately normal to the plane of the two dmg groups.

[b]The entry marked with an asterisk contains Hdpg rather than Hdmg and the distance under $C-CH_3$ is $C-C_6H_5$.

[c]The values given in parentheses are usually the mean of the estimated standard deviations. They are presented only to indicate the precision of the original vaules in a most general sense.

[d]C-py is a carbon-bonded pyridine and DDT is 1,1-bis(4-chlorophenyl)-2-chloroethylene.

Table 19 - extended

X	Y	C-N	C-C	$C-CH_3$	O…O	Reference
clan	Cℓ	1.297(8)	1.463(9)	1.490(11)	2.488(7)	-
clan	clan	1.295(3)	1.477(4)	1.484(4)	2.495(3)	-
*clan	Cℓ	1.309(16)	1.469(16)	1.486(17)	2.500(12)	-
sulfa	Cℓ	1.291(14)	1.471(17)	1.498(17)	2.493(11)	46
NH_3	Cℓ	1.282(4)	1.483(6)	1.50 (2)	2.486(7)	40
tpp	Cℓ	1.300(14)	1.485(15)	1.501(8)	2.50 (1)	40
$SbPh_3$	Cℓ					49
an	an	1.294(6)	1.463(7)	1.479(12)	2.491(8)	52
CH_3	H_2O	1.302(5)	1.463(7)	1.494(7)	2.486(4)	51
C-py	P(n-But)$_3$	1.295(7)	1.443(3)	1.499(3)	2.474(2)	48
CH_2COOCH_3	py	1.28	1.46	1.50	2.50	47
DDT	py	1.30 (2)	1.43 (2)		2.50 (11)	50

ligand as are presented here.

In comparing $C\ell Co(H_2dpg_2)$(clan) with $C\ell Co(H_2dmg)$(dmg)(clan) the distances from the cobalt atom to the equatorial nitrogens in the H_2dpg complex are longer and the distances to the axial ligands are shorter in the same complex. Because the phenyl substituents are inductively more electron withdrawing than methyl groups, Hdpg should be a weaker Lewis base than Hdmg. The equatorial distances to the Hdpg should, therefore, be longer. From an electronic standpoint the cobalt ion in the Hdpg complex would be more positively charged and a better Lewis acid toward the axial ligands than in the Hdmg complex. From a steric point of view the axial ligands are afforded a wider path of approach and will, therefore, be closer to the central cobalt ion when the equatorial ligands are farther away.

The benzene rings in the clan ligands of $C\ell Co(H_2dmg_2)$-(clan), $C\ell Co(H_2dpg_2)$(clan), and $[Co(Hdmg)_2(clan)_2]C\ell$ are planar (see Tables 14-16) having average C-C values of 1.376(3), 1.380(10), and 1.378(3) Å, respectively, with individual values reported in Table 20. The phenyl rings of the Hdpg ligands of $C\ell Co(H_2dpg_2)$(clan) are also planar with pertinent values and equations of least-squares planes given in Table 21.

The crystals of $C\ell Co(H_2dmg)$(dmg)(clan) are held together by six hydrogen bonds where there are eight hydrogen atoms capable of hydrogen bonding. Relevant hydrogen-bonding data are presented in Table 17. Although the O-H···O bridges between the H_2dmg and dmg groups are not symmetrical, the O-H

Table 20

Bond Distances and Bond Angles of Coordinated 4-Chloroaniline Molecules with Their Estimated Standard Deviations.

Distances (Å)	$C\ell Co(H_2dmg_2)(clan)$	$C\ell Co(H_2dpg_2)(clan)$	$[Co(H_2dmg_2)(clan)_2]C\ell$
N(1)-C(1)	1.461([illegible])	1.451(16)	1.443(3)
C(1)-C(2)	1.374(3)	1.380(19)	1.383(4)
C(2)-C(3)	1.364(10)	1.409(20)	1.377(4)
C(3)-C(4)	1.370(10)	1.362(20)	1.364(5)
C(4)-C(5)	1.388(10)	1.344(21)	1.378(6)
C(5)-C(6)	1.378(10)	1.376(20)	1.385(4)
C(6)-C(1)	1.379(9)	1.406(17)	1.380(4)
Cℓ(2)-C(4)	1.734(8)	1.724(15)	1.752(3)
Angles (°)			
N(1)-C(1)-C(2)	119.4(5)	122.0(12)	119.4(2)
N(1)-C(1)-C(6)	119.2(5)	120.7(11)	121.0(2)
C(1)-C(2)-C(3)	119.7(6)	122.4(13)	120.2(3)
C(2)-C(3)-C(4)	119.8(7)	117.9(13)	119.5(3)
C(3)-C(4)-C(5)	120.7(7)	120.8(14)	121.8(4)
C(4)-C(5)-C(6)	119.7(7)	122.3(14)	118.4(3)
C(5)-C(6)-C(1)	118.7(6)	119.4(12)	120.7(3)
C(6)-C(1)-C(2)	121.4(6)	117.2(12)	119.5(2)
Cℓ(2)-C(4)-C(3)	120.5(6)	117.7(11)	119.4(3)
Cℓ(2)-C(4)-C(5)	118.8(6)	121.3(11)	118.8(3)

Table 21

Bond Distances, Bond Angles, and Least-Squares Planes of the Phenyl Rings in $C\ell Co(H_2dpg_2)$(clan) with Their Estimated Standard Deviations.

(a) Distances	n = 13 ℓ = A	14 B	23 C	24 D
C(n)-C(1ℓ)	1.363(18)	1.411(20)	1.370(19)	1.426(17)
C(n)-C(5ℓ)	1.421(20)	1.396(20)	1.356(17)	1.458(18)
C(1ℓ)-C(2ℓ)	1.368(19)	1.371(20)	1.432(19)	1.385(19)
C(2ℓ)-C(3ℓ)	1.370(21)	1.367(20)	1.351(21)	1.401(20)
C(3ℓ)-C(4ℓ)	1.352(20)	1.391(23)	1.371(23)	1.397(20)
C(4ℓ)-C(5ℓ)	1.374(20)	1.390(20)	1.409(18)	1.397(18)
(b) Angles (°)				
C(n-2)-C(n)-C(1ℓ)	123.9(11)	119.3(12)	120.9(11)	121.7(11)
C(n-2)-C(n)-C(5ℓ)	119.9(11)	120.9(12)	121.2(11)	120.6(11)
C(n)-C(1ℓ)-C(2ℓ)	122.8(13)	120.6(13)	122.3(12)	122.6(12)
C(1ℓ)-C(2ℓ)-C(3ℓ)	119.5(13)	119.3(14)	117.0(13)	117.7(13)
C(2ℓ)-C(3ℓ)-C(4ℓ)	120.5(13)	121.0(14)	122.2(14)	122.5(13)
C(3ℓ)-C(4ℓ)-C(5ℓ)	120.0(14)	120.4(14)	118.7(13)	120.2(13)
C(4ℓ)-C(5ℓ)-C(n)	121.0(13)	118.4(14)	121.7(12)	119.0(12)
C(5ℓ)-C(n)-C(1ℓ)	116.2(12)	119.8(13)	117.9(12)	117.7(11)

(c) Deviations ($\mathring{A} \times 10^{+3}$) from Least-Squares Planes of Phenyl Rings

C(n)	2	41	-3	3
C(1ℓ)	-7	-14	8	-12
C(2ℓ)	10	-31	15	24
C(3ℓ)	-10	48	-29	-28
C(4ℓ)	5	-20	3	20
C(5ℓ)	-2	-24	19	-7
C(n-2)	-3	172	-16	20

(d) Coefficients of the Plane Equation PX + QY + RZ = S

	P	Q	R	S
Phenyl A	-0.5815	0.5296	-0.6176	4.7459
Phenyl B	-0.4144	-0.7611	0.4990	3.1793
Phenyl C	-0.6482	0.3950	-0.6509	4.0341
Phenyl D	-0.1592	-0.8986	0.4088	1.3642

distances are longer than might be expected. The two hydrogen atoms on N(1) of the clan ligand both hydrogen bond to different water molecules. The hydrogen atoms of one water molecule, O(w2), form reasonably strong hydrogen bonds to O(12) and Cℓ(1). The hydrogen atoms on O(w1), however, have only short contacts with angles indicating only weak hydrogen bonds.

While $[Co(Hdmg)_2(clan)_2]Cℓ$ and $CℓCo(H_2dpg_2)(clan)$ both exhibit the hydrogen bonding between the equatorial ligands, $CℓCo(H_2dpg_2)(clan)$ has no intermolecular hydrogen bonds. While the hydrogen atom on the solvent molecule was not located, a hydrogen bond may exist between O(S1) and O(22). Each molecule of $[Co(Hdmg)_2(clan)_2]Cℓ$ possesses two intermolecular hydrogen bonds. Each clan molecule shows a hydrogen bond from N(1) to the O(11) of another molecule. The other hydrogen on each N(1) is hydrogen bonded to the ionic chloride. Relevant hydrogen-bonding data for these two compounds are also presented in Table 17.

All intermolecular distances less then 3.6 Å were calculated and carefully examined. No unusually short intermolecular distances were found.

Ligand-induced proton shifts may be of biological significance. Since proton transfers in living systems are relatively common, the study presented here provides an important examination of orientation effects and enhanced stabilities which may be achieved by a small shift of one proton.

CHAPTER 5

A NOVEL BINUCLEATING LIGAND: THE CRYSTAL AND MOLECULAR STRUCTURES OF 1,4-DIHYDRAZINOPHTHALAZINEBIS(2-PYRIDINIUMCARBOXALDIMINE) NITRATE DIHYDRATE AND μ-CHLOROTETRAAQUA[1,4-DIHYDRAZINOPHTHALAZINEBIS(2-PYRIDINECARBOXALDIMINE)]DINICKEL(II) CHLORIDE DIHYDRATE

Binuclear complexes of chelating ligands have been of interest recently for their potential activation of other ligands at an accessible bridging site[68-73] and for their magnetic properties.[24,74-80] The structure of $[Ni_2C\ell(H_2O)_4(dhphpy)]C\ell_3$ shows the planar chelating ligand, dhphpy, to be capable of binding two metal atoms simultaneously. In that complex, a bridging site between the nickel ions is occupied by a chloride ion. Therefore, at least one bridging ligand in addition to dhphpy may be accommodated by M_2dhphpy complexes.

While the study of magnetic interactions between metal ions through bridging atoms in such systems is convenient and theoretically significant, the catalytic possibilities of this type system are exceptional. The nitrogen-fixing enzyme nitrogenase has been considered to contain a polynuclear active site.[6,7]

Although the mechanism of the reduction of N_2 to NH_3 by nitrogenase is not understood N_2 is believed to be coordinated to the metal ions of the enzyme.[67,81,82] Nitrogenase has been shown to reduce a wide variety of small molecules which contain a triple bond.[7] The distance between the metal

ions should be of importance in the activation of those molecules. In the complexes of Robson and coworkers[68-73] and of Okawa et al.[83] the metal-metal distance is essentially controlled by a single bridging phenoxide ion. However, in dhphpy complexes the metal ion separation is fixed at a greater distance by the geometry of the chelating ligand. Therefore, larger molecules which are reduced in the presence of nitrogenase, e.g. N_2, N_3^-, N_2O, C_2H_2, and HCN,[7] should be suitable for incorporation as bridging molecules opposite the N-N bridge of dhphpy. The syntheses and X-ray structures of H_2dhphpy$(NO_3)_2 \cdot H_2O$ and $[Ni_2C\ell(H_2O)_4$(dhphpy)$]C\ell_3 \cdot 2H_2O$ were undertaken to examine the nature of the accessible bridging site in complexes of this type ligand.

Solution and Refinement of the Structure of H_2dhphpy$(NO_3)_2 \cdot 2H_2O$

The direct method of symbolic addition was used in which the signs of two hundred large E's were assigned. All fourteen nonhydrogen atoms of the ligand within the asymmetric unit were located in an E-map computed from the signed E values. Two Fourier syntheses were used to validate the selected model, locate the remaining nonhydrogen atoms, and refine the atomic parameters. The refinement is outlined in Table 5. The observed and calculated structure factors are given in Table B-3. The final positional and thermal parameters are presented in Tables 22 and 23.

Table 22

Final Atomic Parameters[a] for the Nonhydrogen Atoms for $H_2dhphpy(NO_3)_2 \cdot 2H_2O$

Atom	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
C(1)	378(2)	3536(3)	1603(3)	21(1)	80(4)	76(4)	0(3)	6(3)	-6(6)
C(2)	181(2)	2379(3)	2019(3)	21(1)	71(3)	83(4)	-1(3)	5(3)	8(6)
C(3)	354(2)	1293(3)	1534(3)	33(1)	74(4)	110(4)	3(3)	36(4)	-14(7)
C(4)	172(2)	240(3)	2015(4)	39(2)	73(4)	140(5)	-2(4)	43(4)	-13(7)
C(10)	1382(2)	4771(3)	-289(3)	24(1)	97(4)	86(4)	-1(3)	27(3)	-11(6)
C(11)	1579(2)	5947(3)	-658(3)	20(1)	86(4)	91(4)	-7(3)	9(3)	0(6)
C(12)	1968(2)	6072(4)	-1546(4)	27(1)	113(4)	108(4)	-8(4)	35(4)	2(7)
C(13)	2116(2)	7214(4)	-1912(4)	30(1)	142(5)	119(5)	-13(4)	43(4)	36(8)
C(14)	1883(2)	8189(4)	-1367(4)	30(1)	114(5)	148(5)	-15(4)	31(4)	44(8)
C(15)	1521(2)	8013(3)	-457(4)	28(1)	92(4)	140(5)	-9(4)	23(4)	8(8)
N(1)	200(1)	4549(2)	2064(2)	23(1)	77(3)	89(3)	4(3)	25(2)	-7(5)
N(2)	783(1)	3597(2)	753(3)	30(1)	77(3)	99(3)	-9(3)	36(3)	-6(5)
N(3)	972(1)	4712(2)	448(2)	25(1)	73(3)	95(3)	-4(3)	25(3)	1(5)
N(10)	1368(1)	6918(3)	-123(3)	27(1)	81(3)	111(3)	-5(3)	23(3)	7(5)
N(20)	1628(2)	1394(3)	-731(4)	68(2)	93(4)	223(6)	33(4)	148(5)	9(7)
O(1)	565(2)	6955(3)	1629(3)	53(1)	113(3)	162(4)	14(3)	62(3)	-50(6)
O(20)	1843(2)	1108(4)	-1701(5)	114(2)	169(5)	445(9)	15(5)	355(8)	-29(10)
O(21)	1086(2)	1953(3)	-974(3)	58(1)	123(3)	151(4)	34(3)	76(4)	-26(6)
O(22)	1861(2)	1062(4)	290(4)	89(2)	284(7)	285(7)	127(6)	56(6)	109(11)

[a]All values are x 10^4. The estimated standard deviations are given in parentheses. The temperature factors are of the form: $\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}\ell^2 + \beta_{12}hk + \beta_{13}h\ell + \beta_{23}k\ell)]$

Table 23

Final Parameters for the Hydrogen Atoms in $H_2dhphpy(NO_3)_2 \cdot 2H_2O$[a]

Atom [Bonded to]	Distance	x	y	z	B
H(1)[O(1)]	0.78(5)	57(3)	629(4)	185(5)	12.5(1.5)
H(2)[O(1)]	0.88(4)	80(2)	737(4)	228(4)	10.1(1.3)
H(3)[C(3)]	1.00(3)	61(2)	129(3)	84(3)	6.2(0.9)
H(4)[C(4)]	1.01(4)	33(2)	-54(4)	171(3)	8.0(1.1)
H(10)[C(10)]	1.05(4)	157(2)	402(3)	-68(3)	6.5(1.0)
H(12)[C(12)]	1.02(3)	212(2)	533(3)	-196(3)	5.7(0.9)
H(13)[C(13)]	0.99(4)	235(2)	734(4)	-262(4)	9.4(1.3)
H(14)[C(14)]	0.91(4)	200(2)	895(4)	-152(4)	7.9(1.1)
H(15)[C(15)]	1.00(4)	136(2)	870(3)	-1(3)	6.6(1.0)
H(N2)[N(2)]	0.95(4)	85(2)	293(4)	26(4)	9.4(1.2)
H(PY)[N(10)]	1.21(6)	105(3)	682(5)	69(5)	15.9(1.8)

[a]The hydrogen atom is given followed by the atom to which it is bonded in brackets, the corresponding bond distance (in Å), the positional parameters (x 10^{+3}), and the isotropic thermal parameter (in $Å^2$). The estimated standard deviations are given in parentheses.

Solution and Refinement of the Structure of $[Ni_2C\ell(H_2O)_4(dhphpy)]C\ell_3 \cdot 2H_2O$

The position of Ni(1) was determined from a sharpened three-dimensional Patterson function. The positions of the remaining atoms were determined in a manner analogous to that used with $C\ell Co(H_2dmg)(dmg)(clan)$. After the hydrogen atoms were located they were included in further refinement with each having an isotropic thermal parameter one unit higher than the refined isotropic value for the atom to which the hydrogen atom was bonded. A summary of the refinement is given in Table 5. The scattering factors for the nonhydrogen atoms were from Hanson et al.[29] and the hydrogen scattering factors from Stewart et al.[30] Lists of observed and calculated structure factors are given in Table B-4. The final positional and thermal parameters are listed in Tables 24 and 25.

Results and Discussion

The atomic numbering and thermal ellipsoids of $H_2dhphpy \cdot (NO_3)_2 \cdot 2H_2O$ are shown in Figure 6 and those of $[Ni_2C\ell(H_2O)_4(dhphpy)]C\ell_3 \cdot 2H_2O$ are shown in Figure 7. Selected interatomic distances of both compounds are listed in Table 26 and corresponding angles are given in Tables 27 and 28. Both compounds crystallize with the cationic complexes, their anions, and water molecules linked in a three-dimensional hydrogen-bonded network. The postulated hydrogen bonds in the structures are listed in Table 29. Diagrams illustrating the pack-

Table 24
The Final Atomic Parameters[a] of the Nonhydrogen Atoms for $[Ni_2C\ell(H_2O)_4(dhphpy)]C\ell_3 \cdot 2H_2O$

Atom	x	y	z	β_{11}
Ni(1)	11817(7)	17289(5)	9891(3)	442(5)
Ni(2)	11346(6)	-4660(5)	13854(3)	407(5)
Cℓ(1)	1046(1)	315(1)	650(1)	63(1)
Cℓ(2)	1196(2)	4767(1)	2115(1)	86(2)
Cℓ(3)	1297(2)	-1548(1)	3350(1)	69(1)
Cℓ(4)	1288(2)	3725(2)	4540(1)	90(2)
O(1)	-362(4)	1864(3)	639(2)	55(3)
O(2)	2743(4)	1634(3)	1329(2)	55(3)
O(3)	-423(3)	-532(3)	1026(2)	48(3)
O(4)	2664(3)	-435(4)	1708(2)	48(3)
O(5)	1626(4)	-520(4)	-194(2)	54(3)
O(6)	1072(4)	5047(5)	3678(2)	74(4)
N(1)	1178(4)	1408(3)	1690(2)	50(4)
N(2)	1153(4)	576(3)	1834(2)	48(4)
N(3)	1265(4)	2854(3)	1801(2)	74(5)
N(4)	1258(4)	2873(3)	1324(2)	53(4)
N(5)	1143(4)	-469(3)	2395(2)	55(4)
N(6)	1165(4)	-1007(3)	2025(2)	45(4)
N(10)	1234(4)	2554(4)	433(2)	54(4)
N(20)	1163(4)	-1776(4)	1227(2)	55(4)
C(1)	1233(5)	2052(4)	1992(3)	42(4)
C(2)	1251(5)	1919(4)	2495(3)	36(4)
C(3)	1280(5)	2594(5)	2826(3)	50(5)
C(4)	1300(5)	2410(5)	3302(3)	56(5)
C(5)	1288(5)	1559(5)	3450(3)	51(5)
C(6)	1260(5)	887(4)	3136(2)	47(5)
C(7)	1236(4)	1057(4)	2649(2)	29(4)
C(8)	1182(4)	394(4)	2288(2)	29(4)
C(10)	1281(6)	3550(4)	1076(3)	71(6)
C(11)	1291(5)	3337(5)	578(3)	52(5)

Table 24- extended

β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
273(4)	106(1)	-66(8)	224(5)	14(4)
244(3)	92(1)	2(8)	184(4)	13(4)
31(1)	10(0)	-10(2)	26(1)	-2(1)
35(1)	14(0)	8(2)	18(1)	0(1)
50(1)	17(0)	46(2)	39(1)	17(1)
72(1)	25(1)	-58(3)	26(2)	-1(1)
42(3)	21(1)	3(5)	26(3)	6(3)
40(2)	21(1)	-6(5)	29(3)	2(3)
58(3)	18(1)	-5(5)	23(3)	22(3)
69(3)	12(1)	17(5)	14(3)	-2(3)
62(3)	17(1)	1(5)	26(3)	-3(3)
111(5)	18(1)	1(7)	35(4)	-6(4)
23(2)	11(1)	-2(5)	25(3)	-1(2)
24(2)	11(1)	-1(5)	25(3)	1(2)
26(2)	15(1)	-14(6)	38(4)	-3(3)
31(3)	14(1)	-12(5)	29(3)	3(3)
25(2)	9(1)	1(5)	19(3)	1(2)
26(2)	11(1)	-1(5)	21(3)	3(2)
41(3)	14(1)	5(5)	33(3)	10(3)
32(3)	13(1)	13(5)	26(3)	0(3)
24(3)	14(1)	-9(6)	26(4)	0(3)
30(3)	13(1)	-11(6)	14(4)	-6(3)
37(4)	14(1)	-12(7)	27(4)	-10(3)
44(4)	14(1)	-8(7)	26(4)	-17(4)
55(4)	12(1)	-17(7)	23(4)	-11(4)
40(4)	9(1)	-2(6)	18(4)	1(3)
32(3)	10(1)	-8(6)	15(4)	-3(3)
28(3)	12(1)	-5(6)	20(3)	-2(3)
30(3)	20(2)	-7(7)	41(5)	7(4)
36(3)	17(1)	-3(7)	29(4)	7(4)

Table 24 - continued

Atom	x	y	z	β_{11}
C(12)	1343(6)	4055(5)	270(3)	83(7)
C(13)	1353(7)	3839(6)	-202(3)	86(7)
C(14)	1308(6)	2992(6)	-348(3)	73(6)
C(15)	1251(6)	2361(5)	-17(3)	59(6)
C(20)	1143(5)	-1829(4)	2053(3)	54(5)
C(21)	1147(5)	-2273(4)	1604(3)	48(5)
C(22)	1149(6)	-3175(5)	1577(3)	64(6)
C(23)	1165(6)	-3554(5)	1149(3)	77(6)
C(24)	1204(6)	-3048(5)	758(3)	76(6)
C(25)	1195(5)	-2157(5)	812(3)	55(5)

[a]All values are x 10^4 except for those of Ni(1) and Ni(2) which are x 10^5. The estimated standard deviations are given in parentheses. The temperature factors are of the form: $\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}\ell^2 + \beta_{12}hk + \beta_{13}h\ell + \beta_{23}k\ell)]$

Table 24 - extended - continued

β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
49(4)	20(2)	-19(9)	36(6)	19(4)
68(5)	17(2)	-27(10)	34(6)	21(5)
68(5)	20(2)	7(9)	47(6)	15(5)
60(5)	14(1)	-6(8)	27(5)	5(4)
29(3)	14(1)	0(6)	29(4)	6(3)
31(3)	14(1)	10(6)	25(4)	5(3)
32(3)	21(2)	6(7)	31(5)	3(4)
39(4)	21(2)	15(8)	33(5)	-6(4)
43(4)	19(2)	8(8)	24(5)	-13(4)
39(4)	16(1)	2(7)	24(5)	-6(4)

Table 25

Final Parameters for the Hydrogen Atoms in $[Ni_2Cl(H_2O)_6(dhphpy)]Cl_3 \cdot 2H_2O$[a]

Atom [Bonded to]	Distance	x	y	z	B
H(N3) [N(3)]	0.91	1397	3365	1972	4.6
H(N5) [N(5)]	0.97	1394	-703	2742	3.8
H(C3) [C(3)]	1.09	1271	3289	2781	4.8
H(C4) [C(4)]	1.05	1323	2949	3525	4.9
H(C5) [C(5)]	0.99	1316	1515	3799	4.8
H(C6) [C(6)]	1.02	1283	313	3312	4.2
H(10) [C(10)]	1.06	1379	4129	1286	5.0
H(12) [C(12)]	1.15	1514	4705	486	6.0
H(13) [C(13)]	1.10	1428	4364	-441	6.6
H(14) [C(14)]	1.04	1443	2797	-657	6.2
H(15) [C(15)]	1.04	1025	1751	-172	4.6
H(20) [C(20)]	1.05	993	-2163	2330	4.5
H(22) [C(22)]	1.04	1197	-3492	1907	5.3
H(23) [C(23)]	1.02	1313	-4180	1103	5.8
H(24) [C(24)]	1.17	972	-3299	327	6.4
H(25) [C(25)]	1.18	1233	-1547	576	5.4
H(1) [O(1)]	1.12	-708	1312	372	5.6
H(1') [O(1)]	0.95	-494	2465	576	5.6
H(2) [O(2)]	0.84	3145	1240	1479	5.5

Table 25 - continued

Atom [Bonded to]	Distance	x	y	z	B
H(2')[O(2)]	1.00	3228	2098	1520	5.5
H(3)[O(3)]	0.91	-793	-51	891	5.6
H(3')[O(3)]	0.73	-688	-756	1149	5.6
H(4)[O(4)]	0.92	3049	-428	2060	5.4
H(4')[O(4)]	0.85	2808	-935	1646	5.4
H(5)[O(5)]	0.86	1353	-476	14	5.7
H(5')[O(5)]	0.90	2283	-622	-50	5.7
H(6)[O(6)]	1.15	863	4328	3630	7.4
H(6')[O(6)]	1.13	1345	4724	4067	7.4

[a]The hydrogen atom is given followed by the atom to which it is bonded in brackets, the corresponding bond distance (in Å), the positional parameters (x 10^{+3}), and the isotropic thermal parameter (in $Å^2$).

Figure 6

An ORTEP drawing of $H_2dhphpy(NO_3)_2 \cdot 2H_2O$ showing the atomic numbering and thermal ellipsoids. The hydrogen atoms are isotropic and small relative to the 50% probability thermal ellipsoids for nonhydrogen atoms.

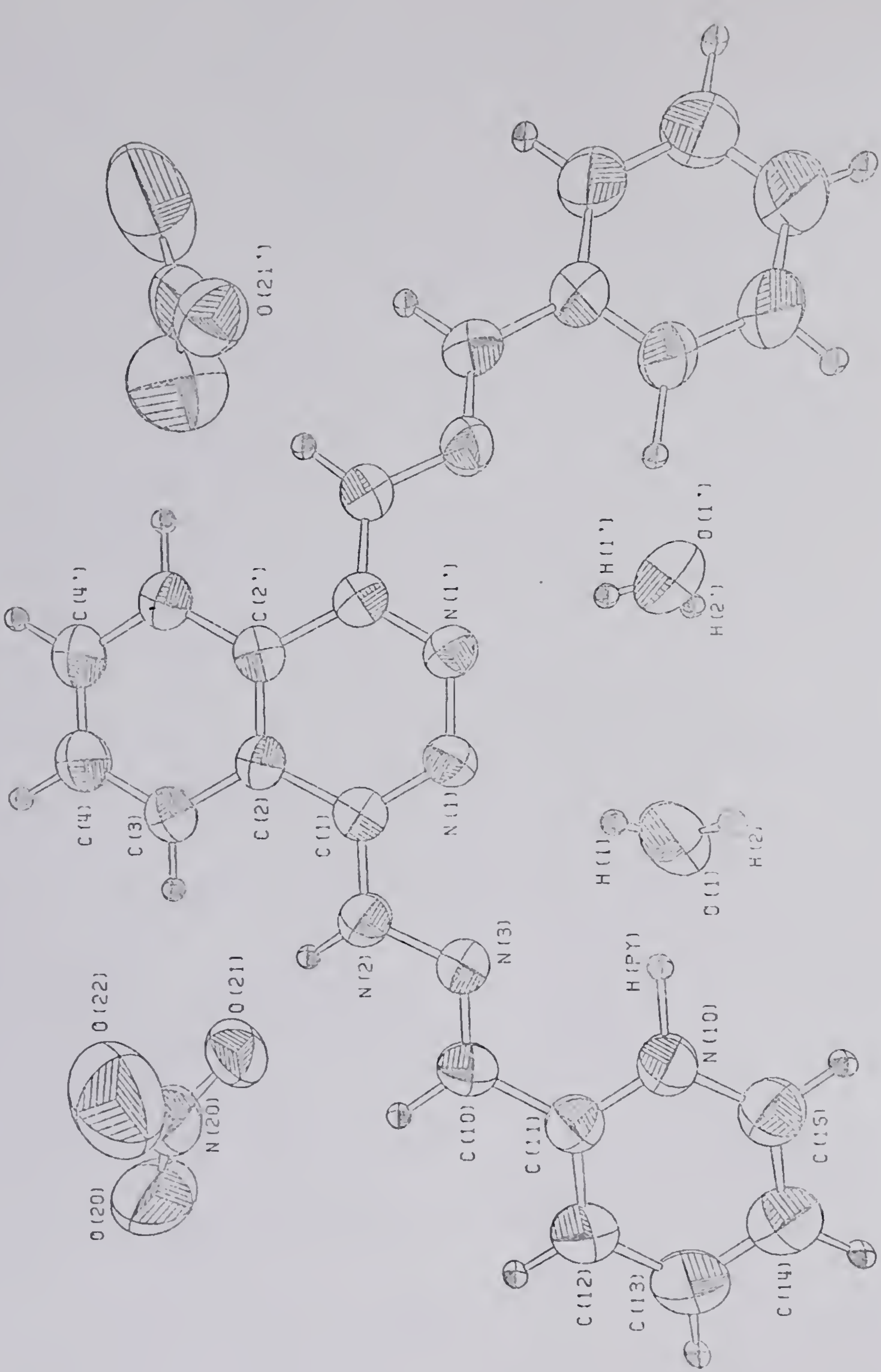
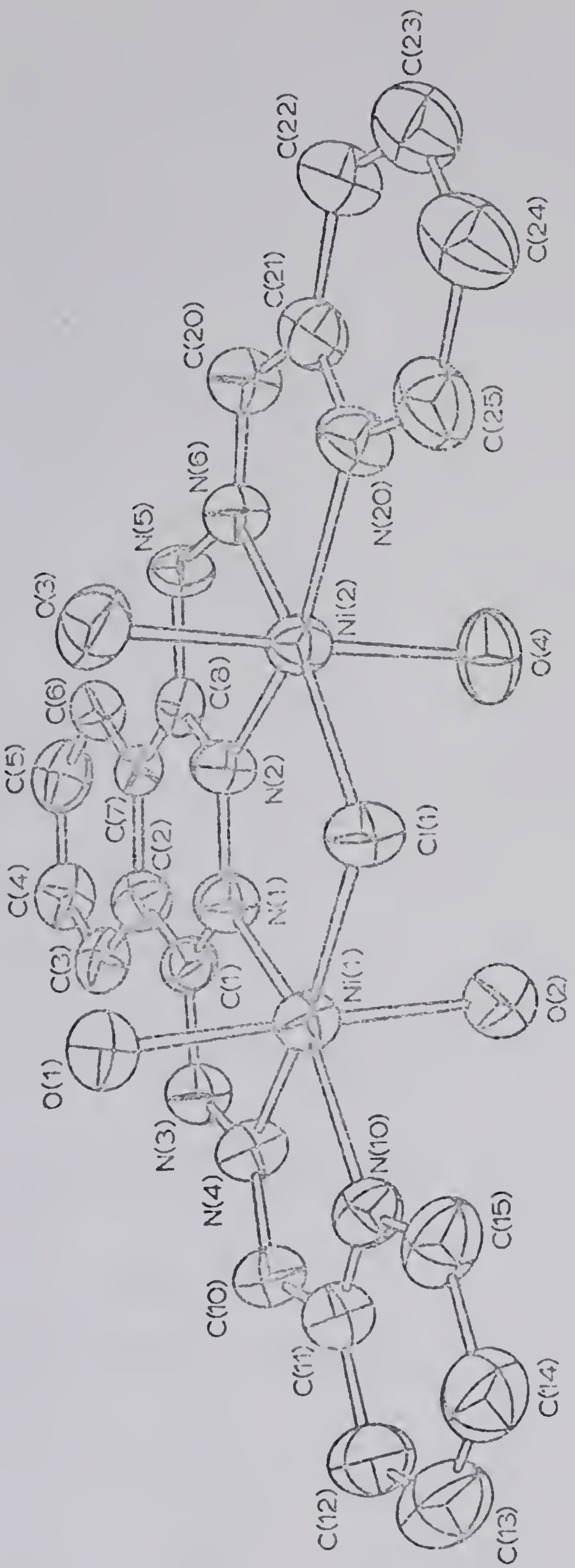

O(21')
C(4')
C(2')
N(1')
H(1')
O(1')
H(2')
C(4)
C(3)
C(2)
C(1)
N(1)
H(1)
O(1)
H(2)
O(22)
O(21)
N(2)
N(3)
H(PY)
N(10)
N(20)
O(20)
C(10)
C(11)
C(15)
C(12)
C(13)
C(14)

Figure 7

An ORTEP drawing of $[Ni_2C\ell(H_2O)_4(dhphpy)]\cdot 2H_2O$ showing atomic numbering and thermal ellipsoids. The hydrogen atoms and uncoordinated water molecules have been omitted.



C(23)
C(22)
C(24)
C(21)
C(20)
C(25)
N(6)
N(20)
N(5)
C(3)
Ni(2)
O(4)
C(6)
C(8)
C(5)
N(2)
C(7)
C(2)
Cl(1)
C(4)
N(1)
C(3)
C(1)
Ni(1)
O(2)
O(1)
N(3)
N(10)
N(4)
C(15)
C(10)
C(11)
C(14)
C(12)
C(13)

Table 26

Selected Interatomic Distances for $H_2dhphpy(NO_3)_2 \cdot 2H_2O$ and $[Ni_2C\ell(H_2O)_4(dhphpy)]C\ell_3 \cdot 2H_2O$

(a) Distance (Å) in the Coordination Sphere in $[Ni_2C\ell(H_2O)_4(dhphpy)]C\ell_3 \cdot 2H_2O$

Ni(1)-N(1)	2.074(6)	Ni(2)-N(2)	2.061(5)
Ni(1)-N(4)	1.999(5)	Ni(2)-N(6)	2.001(5)
Ni(1)-N(10)	2.074(6)	Ni(2)-N(20)	2.089(6)
Ni(1)-Cℓ(1)	2.374(2)	Ni(2)-Cℓ(1)	2.387(2)
Ni(1)-O(1)	2.098(6)	Ni(2)-O(3)	2.108(6)
Ni(1)-O(2)	2.117(6)	Ni(2)-O(4)	2.070(6)

(b) Distances (Å) within the Ligand[a]

$H_2dhphpy(NO_3)_2 \cdot 2H_2O$		$[Ni_2C\ell(H_2O)_6(dhphpy)]C\ell_3 \cdot 2H_2O$			
N(1)-N(1')	1.374(4)	N(1)-N(2)	1.363(7)		
N(1)-C(1)	1.318(4)	N(1)-C(1)	1.302(8)	N(2)-C(8)	1.313(8)
C(1)-C(2)	1.454(5)	C(1)-C(2)	1.447(10)	C(7)-C(8)	1.439(9)
C(2)-C(3)	1.396(5)	C(2)-C(3)	1.402(10)	C(6)-C(7)	1.407(9)
C(3)-C(4)	1.369(5)	C(3)-C(4)	1.383(10)	C(5)-C(6)	1.368(10)
C(2)-C(2')	1.396(5)	C(2)-C(7)	1.414(9)		
C(4)-C(4')	1.378(6)	C(4)-C(5)	1.390(11)		
C(1)-N(2)	1.362(4)	C(1)-N(3)	1.370(8)	C(8)-N(5)	1.382(8)
N(2)-N(3)	1.366(4)	N(3)-N(4)	1.366(8)	N(5)-N(6)	1.364(7)
N(3)-C(10)	1.277(4)	N(4)-C(10)	1.278(9)	N(6)-C(20)	1.279(8)
C(10)-C(11)	1.454(5)	C(10)-C(11)	1.457(11)	C(20)-C(21)	1.464(10)

Table 26 - continued

H_2dhphpy$(NO_3)_2 \cdot 2H_2O$		$[Ni_2C\ell(H_2O)_6$(dhphpy)$]C\ell_3 \cdot 2H_2O$			
C(11)-C(12)	1.397(5)	C(11)-C(12)	1.388(11)	C(21)-C(22)	1.402(10)
C(12)-C(13)	1.387(6)	C(12)-C(13)	1.400(13)	C(22)-C(23)	1.370(12)
C(13)-C(14)	1.370(6)	C(13)-C(14)	1.373(13)	C(23)-C(24)	1.392(12)
C(14)-C(15)	1.364(6)	C(14)-C(15)	1.392(12)	C(24)-C(25)	1.393(11)
C(15)-N(10)	1.331(5)	C(15)-N(10)	1.339(10)	C(25)-N(20)	1.349(10)
N(10)-C(11)	1.343(4)	N(10)-C(11)	1.351(9)	N(20)-C(21)	1.339(9)
O(1)···N(3)	3.007(4)				
O(1)···O(1')	3.283(4)	Ni(1)···Ni(2)	3.603(1)		

[a]The estimated standard deviations are given in parentheses.

Table 27

Selected Angles in $H_2dhphpy(NO_3)_2 \cdot 2H_2O$[a]

Atoms	Angles (°)	Atoms	Angles (°)
N(1)-C(1)-N(2)	117.9(3)	C(1)-C(2)-C(3)	123.1(3)
N(1)-C(1)-C(2)	121.9(3)	C(2')-C(2)-C(3)	119.7(3)
C(1)-C(2)-C(2')	117.2(3)	C(1)-N(1)-N(1')	120.8(3)
C(2)-C(3)-C(4)	119.4(3)	C(2)-C(1)-N(2)	120.1(3)
C(3)-C(4)-C(4')	120.8(4)	N(2)-N(3)-C(10)	117.2(3)
C(1)-N(2)-N(3)	116.9(3)	C(10)-C(11)-N(10)	118.5(3)
N(3)-C(10)-C(11)	118.4(3)	C(11)-C(12)-C(13)	119.0(4)
C(10)-C(11)-C(12)	121.2(3)	C(13)-C(14)-C(15)	119.1(4)
C(12)-C(13)-C(14)	119.5(4)	C(14)-C(15)-N(10)	121.5(4)
C(15)-N(10)-C(11)	120.6(3)	N(10)-C(11)-C(12)	120.3(3)
N(1)···O(1)···N(10)	108.3(1)	O(20)-N(20)-O(21)	118.1(4)
N(20)-O(21)···N(2)	123.0(3)	O(20)-N(20)-O(22)	123.9(5)
O(21)-N(20)-O(22)	117.6(4)		

[a]The estimated standard deviations are given in parentheses.

Table 28

Selected Angles in $[Ni_2C\ell(H_2O)_6(dhphpy)]C\ell_3 \cdot 2H_2O$[a]

Atom	Angle	Atom	Angle
N(1)-Ni(1)-Cℓ(1)	98.0(2)	N(2)-Ni(2)-Cℓ(1)	97.8(2)
N(1)-Ni(1)-N(4)	76.8(2)	N(2)-Ni(2)-N(6)	76.5(2)
N(1)-Ni(1)-N(10)	155.7(2)	N(2)-Ni(2)-N(20)	154.8(2)
N(1)-Ni(1)-O(1)	91.1(2)	N(2)-Ni(2)-O(3)	93.1(2)
N(1)-Ni(1)-O(2)	90.3(2)	N(2)-Ni(2)-O(4)	89.5(2)
N(4)-Ni(1)-Cℓ(1)	174.6(2)	N(6)-Ni(2)-Cℓ(1)	174.1(2)
N(4)-Ni(1)-N(10)	78.9(2)	N(6)-Ni(2)-N(20)	78.2(2)
N(4)-Ni(1)-O(1)	87.8(2)	N(6)-Ni(2)-O(3)	90.4(2)
N(4)-Ni(1)-O(2)	91.1(2)	N(6)-Ni(2)-O(4)	91.2(2)
N(10)-Ni(1)-Cℓ(1)	106.3(2)	N(20)-Ni(2)-Cℓ(1)	107.5(2)
N(10)-Ni(1)-O(1)	88.5(2)	N(20)-Ni(2)-O(3)	88.3(2)
N(10)-Ni(1)-O(2)	89.6(2)	N(20)-Ni(2)-O(4)	89.8(2)
O(1)-Ni(1)-Cℓ(1)	90.9(2)	O(3)-Ni(2)-Cℓ(1)	88.2(2)
O(1)-Ni(1)-O(2)	178.0(2)	O(3)-Ni(2)-O(4)	177.2(2)
O(2)-Ni(1)-Cℓ(1)	90.3(2)	O(4)-Ni(2)-Cℓ(1)	90.5(2)
N(10)-C(11)-C(12)	122.2(7)	N(20)-C(21)-C(22)	121.9(7)
C(11)-C(12)-C(13)	117.8(8)	C(21)-C(22)-C(23)	118.7(7)
C(12)-C(13)-C(14)	120.3(9)	C(22)-C(23)-C(24)	120.2(8)
C(13)-C(14)-C(15)	118.4(8)	C(23)-C(24)-C(25)	117.7(8)
C(14)-C(15)-N(10)	122.3(8)	C(24)-C(25)-N(20)	122.6(7)
C(15)-N(10)-C(11)	119.1(7)	C(25)-N(20)-C(21)	118.8(6)
N(10)-C(11)-C(10)	116.2(7)	N(20)-C(21)-C(20)	116.7(6)
C(12)-C(11)-C(10)	121.6(7)	C(22)-C(21)-C(20)	121.4(7)
C(11)-C(10)-N(4)	114.7(7)	C(21)-C(20)-N(6)	113.8(6)
C(10)-N(4)-N(3)	125.9(6)	C(20)-N(6)-N(5)	123.4(6)
N(4)-N(3)-C(1)	115.8(6)	N(6)-N(5)-C(8)	113.8(5)
N(1)-C(1)-N(3)	115.7(6)	N(2)-C(8)-N(5)	116.3(6)
C(2)-C(1)-N(3)	122.7(6)	C(7)-C(8)-N(5)	121.8(6)
N(1)-C(1)-C(2)	121.6(6)	N(2)-C(8)-C(7)	121.8(6)
C(1)-N(1)-N(2)	121.8(6)	C(8)-N(2)-N(1)	120.8(5)
C(1)-C(2)-C(7)	116.8(6)	C(2)-C(7)-C(8)	117.0(6)

Table 28 - continued

Atom	Angle	Atom	Angle
C(1)-C(2)-C(3)	123.5(6)	C(6)-C(7)-C(8)	123.5(6)
C(2)-C(3)-C(4)	119.7(7)	C(5)-C(6)-C(7)	119.4(6)
C(3)-C(4)-C(5)	120.1(7)	C(4)-C(5)-C(6)	121.6(7)
Ni(1)-N(1)-N(2)	122.4(4)	Ni(2)-N(2)-N(1)	123.3(4)
Ni(1)-N(1)-C(1)	115.8(5)	Ni(2)-N(2)-C(8)	115.9(4)
Ni(1)-N(4)-N(3)	115.9(4)	Ni(2)-N(6)-N(5)	117.3(4)
Ni(1)-N(4)-C(10)	118.2(5)	Ni(2)-N(6)-C(20)	119.1(5)
Ni(1)-N(10)-C(11)	111.9(5)	Ni(2)-N(20)-C(21)	112.1(5)
Ni(1)-N(10)-C(15)	128.9(5)	Ni(2)-N(20)-C(25)	129.1(5)
Ni(1)-Cℓ(1)-Ni(2)	98.4(1)		

[a]The estimated standard deviations are given in parentheses.

Table 29

Hydrogen Bonds in $H_2dhphpy(NO_3)_2 \cdot 2H_2O$ and $[Ni_2C\ell(H_2O)_4(dhphpy)]C\ell_3 \cdot 2H_2O$

D-H···A[a]	Position of A	Distances (Å)[b] D-H	H···A	D···A	Angles (°) D-H···A
$H_2dhphpy(NO_3)_2 \cdot 2H_2O$					
N(2)-H(N2)···O(21)	x,y,z	0.95(4)	1.85(4)	2.773(4)	163(4)
N(10)-H(PY)···O(1)	x,y,z	1.21(6)	1.57(6)	2.758(4)	167(5)
O(1)-H(1)···N(1)	x,y,z	0.78(5)	2.12(5)	2.855(4)	159(5)
O(1)-H(2)···O(21)	x,1-y,1/2+z	0.88(4)	1.98(4)	2.824(4)	160(4)
$[Ni_2C\ell(H_3O)_4(dhphpy)2C\ell_3 \cdot 2H_2O$					
N(3)-H(N3)···Cℓ(2)	x,y,z	0.91	2.26	3.119(6)	158
N(5)-H(N5)···Cℓ(3)	x,y,z	0.97	2.24	3.135(6)	153
O(1)-H(1)···O(5)	-x,-y,-z	1.12	1.75	2.735(8)	144
O(1)-H(1')···Cℓ(4)	-x,y,1/2-z	0.95	2.24	3.150(6)	159
O(2)-H(2')···Cℓ(3)	1/2-x,1/2+y,1/2-z	1.00	2.20	3.121(6)	152
O(3)-H(3')···Cℓ(3)	-x,y,1/2-z	0.73	2.36	3.075(6)	171
O(4)-H(4)···Cℓ(2)	1/2-x,1/2+y,1/2-z	0.92	2.16	3.067(5)	171
O(5)-H(5)···Cℓ(1)	x,y,z	0.86	2.41	3.185(6)	151
O(5)-H(5')···Cℓ(4)	1/2-x,1/2+y,1/2-z	0.90	2.25	3.098(6)	157
O(6)-H(6')···Cℓ(4)	x,y,z	1.23	2.09	3.121(7)	151

[a]Donor-Hydrogen···Acceptor. D-H is at x,y,z.

[b]The estimated standard deviations are given in parentheses.

ing and hydrogen bonding in $H_2dhphpy(NO_3)_2 \cdot 2H_2O$ and in $[Ni_2C\ell(H_2O)_4(dhphpy)]C\ell_3 \cdot 2H_2O$ are presented in Figures 8 and 9.

The most noticeable difference in the structures of the two dhphpy ligands is that $H_2dhphpy(NO_3)_2 \cdot 2H_2O$ contains a twofold rotation axis while the nickel complex does not. In both cases the ligand is approximately planar (see Table 30). The nickel atoms and the bridging chloride of $[Ni_2C\ell(H_2O)_4$-$(dhphpy)]C\ell_3 \cdot 2H_2O$ lie slightly "below" the least-squares plane of the ligand (Plane 3) and both hydrazone portions are pivoted generally about an N(3)···N(5) axis with both C(14) and C(24) "above" the plane. However, in the protonated ligand one hydrazone is pivoted "upward" and the other "downward" as required by the twofold axis. Also, the hydrazone "arms" in the nickel complex are drawn toward each other compared to the protonated form as indicated by the bond angles within the "arms." All of the pyridine rings are rotated about the C(n0)-C(n1) bond relative to the phthalazine plane with the pyridine nitrogen atoms tipped toward the coordinated species. In $[Ni_2C\ell(H_2O)_4(dhphpy)]C\ell_3 \cdot 2H_2O$ the pyridine containing N(10) is rotated to a much greater extent than that containing N(20). This is shown by the deviations from plane 4 (Table 30) of N(10) and C(12), 0.124 and 0.222 Å, compared to the deviations of N(20) and C(22), 0.148 and 0.161 Å. The rings of the phthalazine fragment in each compound appear twisted relative to each other but by less than 2°.

Figure 8

A packing diagram of H_2dhphpy$(NO_3)_2 \cdot 2H_2O$ with atoms at x,y,z and $\bar{x},1-y,1-z$ labeled and those at $x,1-y,1/2+z$ and $\bar{x},y,1/2-z$ unlabeled. Proposed hydrogen bonds are indicated by broken lines.

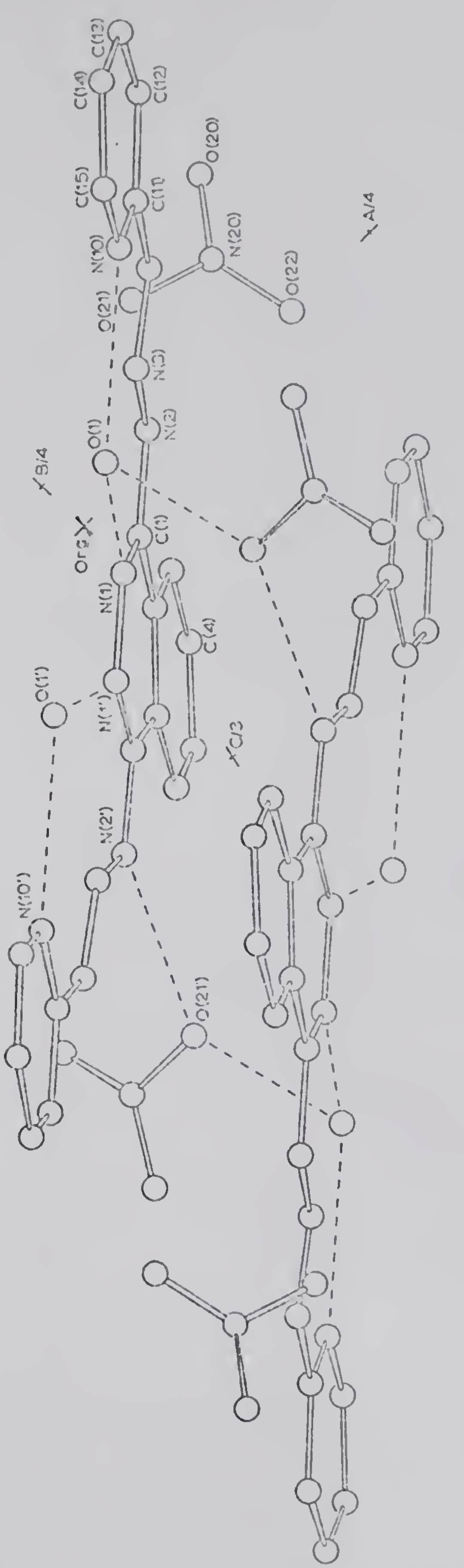

C(13)
C(14)
C(12)
O(20)
C(15)
C(11)
N(10)
N(20)
A/4
O(22)
O(21)
N(3)
N(2)
O(1)
B/4
Org
C(1)
N(1)
C(4)
O(1')
N(1')
C/3
N(2')
N(10')
O(21')

Figure 9

A packing diagram of $[Ni_2C\ell(H_2O)_4(dh\underline{p}hpy)]\cdot 2H_2O$ where O(6) is at x,y,z; O(6') is at $\overline{x},\overline{y},\overline{z}$; O(6") is at 1/2-x,1/2+y,1/2-z; and O(6"') is at 1/2+x,1/2+y,z. Proposed hydrogen bonds are indicated by broken lines.

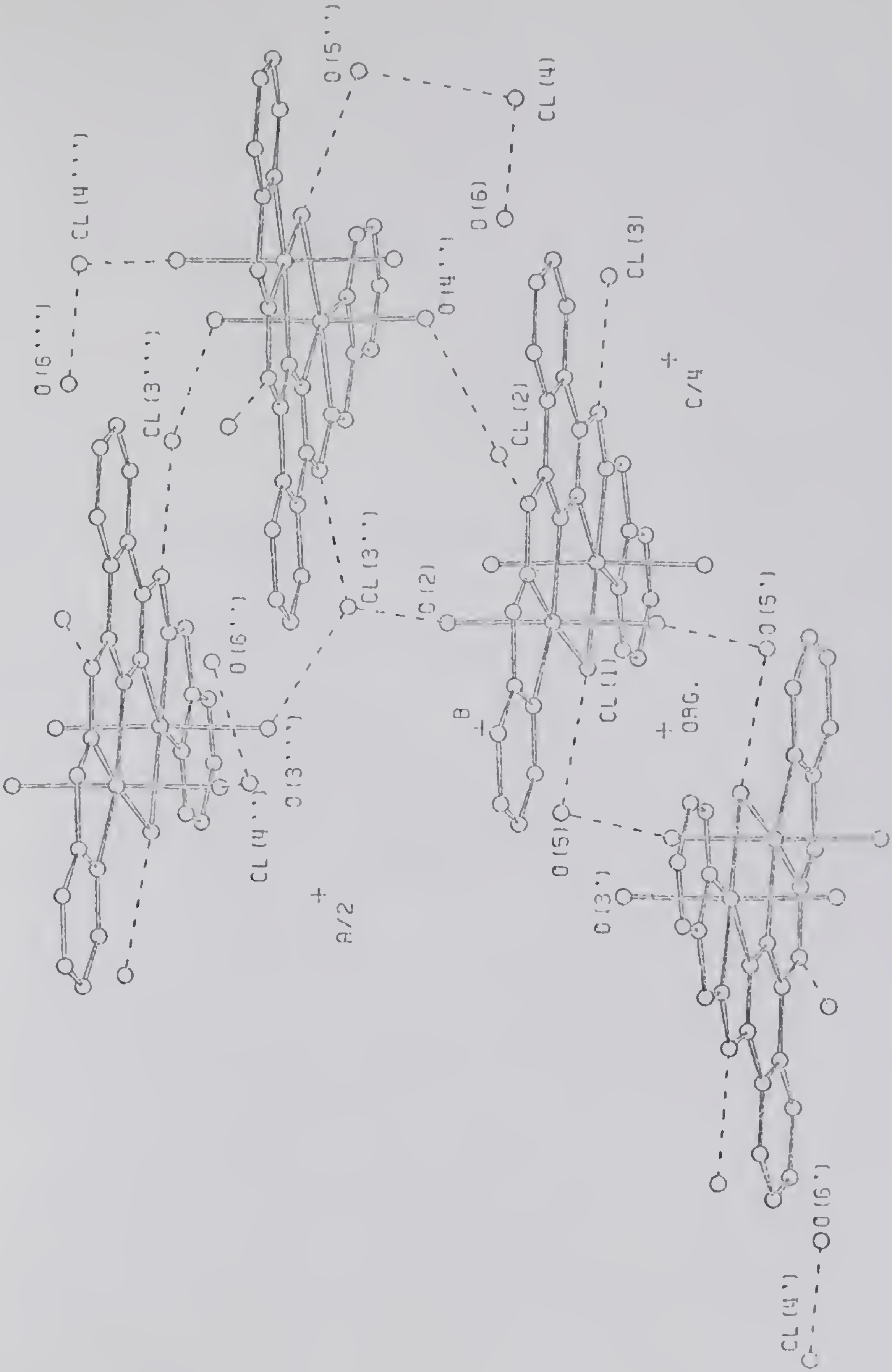

O(5'')
CL(4)
O(6)
CL(4''')
O(6''')
O(4'')
CL(3)
CL(3''')
C/4
CL(2)
CL(3'')
O(2)
O(5')
O(6'')
CL(1)
B
ORG.
O(3''')
CL(4'')
O(5)
A/2
O(3')
O(6')
CL(4')

Table 30

Deviations and Equations of Selected Least-Squares Planes in $H_2dhphpy(NO_3)_2 \cdot 2H_2O$ and $[Ni_2C\ell(H_2O)_4(dhphpy)]C\ell_3 \cdot 2H_2O$

(a) Deviations ($Å \times 10^{-3}$)[a]

$H_2dhphpy(NO_3)_2 \cdot 2H_2O$			$[Ni_2C\ell(H_2O)_4(dhphpy)]C\ell_3 \cdot 2H_2O$					
Atom	Plane 1	Plane 2	Atom	Plane 3	Plane 4	Atom	Plane 3	Plane 4
N(1)	-18*	-2*	N(1)	-85*	-6*	N(2)	-92*	-15*
C(1)	-40*	15*	C(1)	-28*	13*	C(8)	-44*	-5*
C(2)	-2*	-13*	C(2)	6*	8*	C(7)	12*	11*
C(3)	-43*	-14*	C(3)	27*	-8*	C(6)	54*	13*
C(4)	52*	14*	C(4)	63*	-12*	C(5)	74*	-4*
N(2)	-40*	119	N(3)	-9*	43	N(5)	-70*	-30
N(3)	-16*	200	N(4)	-24*	71	N(6)	-27*	53
C(10)	62*	376	C(10)	-14*	94	C(20)	-32*	56
C(11)	53*	429	C(11)	0*	155	C(21)	-18*	117
C(12)	5*	448	C(12)	47*	222	C(22)	13*	161
C(13)	-66*	472	C(13)	63*	283	C(23)	42*	233
C(14)	-63*	424	C(14)	27*	270	C(24)	76*	296
C(15)	36*	418	C(15)	-29*	192	C(25)	38*	242
N(10)	79*	407	N(10)	-54*	124	N(20)	-13*	148
O(1)	116	243	Ni(1)	-95	43	Ni(2)	-90	40
			Cℓ(1)	-239	-55			

Table 30 - continued

(b) Coefficients of the plane equation $AX + BY + CZ = D$[58]

Plane	A	B	C	D
$H_2dhphpy(NO_3)_2 \cdot 2H_2O$				
1	0.6518	-0.0289	0.7578	1.4465
2	0.7079	-0.0175	0.7061	1.3716
$[Ni_2C\ell(H_2O)_4(dhphpy)]C\ell_3 \cdot 2H_2O$				
3	0.8991	-0.0193	0.4374	1.6470
4	0.9121	-0.0276	0.4091	1.4216

[a]The entries marked with an asterisk were used to define the plane.

All bonding distances involving nonhydrogen atoms are normal. The N-N distances in both compounds range from 1.363(7) to 1.374(4) Å and are comparable to the N-N distance in 4-FPYTSC of 1.365(3) Å.[84] Since this distance in both the phthalazine and hydrazone groups is significantly shorter than the accepted N-N single bond distance, 1.44±4 Å,[85] and since the ligand is planar, a delocalized system is presumed to exist. In agreement with this assumption the C(n0)-N distances are longer than the pure C-N double bond distance and are all equivalent to the related C-N distance in 4-FPYTSC, 1.275(3) Å.[84] All other distances within the ligand are not significantly different from those in [Ni(dhph)$(H_2O)_2Cl_4 \cdot 2H_2O$.[86]

All Ni-N distances in $[Ni_2Cl(H_2O)_4(dhphpy)]Cl_3 \cdot 2H_2O$ are within the range of reported bonding distances of nickel(II) with aromatic nitrogen atoms (2.00 to 2.112 Å).[87]

The bridging chloride is not symmetrically located between the two nickel atoms with Ni-Cl distances of 2.374(2) and 2.387(2) Å. The appearance of this bridge is remarkably similar to that in di-μ-chloro-<u>sym</u>-<u>trans</u>-dichlorobis-(2,9-dimethyl-1,10-phenanthroline)dinickel(II) · 2chloroform[88] where the Ni-C distances are 2.378(3) and 2.394(3) Å. Also, the Ni···Ni distance, 3.602(2) Å, and Ni-Cl-Ni angle, 98.0(1)°, in that compound are equivalent to the 3.603(1) Å separation and 98.36(7)° angle in $[Ni_2Cl(H_2O)_6(dhphpy)]Cl_3 \cdot 2H_2O$. This distance between the nickel atoms is somewhat shorter than

the 3.791(4) Å distance found in the $[Ni(dhph)(H_2O_2]_2C\ell_4 \cdot 2H_2O$ complex reported by Andrew and Blake[86] where both bridges are phthalazine nitrogen atoms. The separation between the nickel atoms in the dhphpy complex, however, is substantially longer then the Ni···Ni distance of 2.879 Å in the doubly oxo-bridged complex of Hoskins, Robson, and Schaap.[70] All these inter-nickel distances are much greater than twice the covalent radius of nickel and must be a function of the bridging atoms.

The distorted octahedral coordination geometry about each nickel atom in $[Ni_2C\ell(H_2O)_4(dhphpy)]C\ell_3 \cdot 2H_2O$ is completed by two water molecules which lie on a line almost perpendicular to the ligand plane. The Ni-O bond distances are typical[87] for water coordinated to nickel(II) ranging from 2.070(6) to 2.117(6) Å.

A degree of uncertainty exists concerning the positions of hydrogen atoms about O(1) in $H_2dhphpy(NO_3)_2 \cdot 2H_2O$. The O(1)-H(1) distance appears to be very short, 0.78 Å, while the N(10)-H(py) distance appears to be very long, 1.21 Å. Although the locations presented for the hydrogen atoms are the most reasonable interpretation of the difference map in terms of peak heights, distances, and H-O-H angles, other areas of positive density exist about the N(1), O(1), and N(10) positions. Disorder may exist with alternate forms having N(1) protonated or having a "coordinated hydronium ion."

Complexes of dhphpy structurally provide a promising

uni-molecular system for the incorporation of a small molecule at a bridging position. Dinitrogen has been reported as a bridging ligand connecting two metal complexes in the μ-dinitrogen-bis{[1,2-bis(dimethylphosphino)ethane]hydrido-[η-(1,3,5-trimethylbenzene)]molybdenum} cation and similar compounds.[89] No complex has been reported which could retain its structural integrity after the removal of a bridging dinitrogen. The structures presented here suggest complexes of ligands similar to dhphpy may have such a capacity.

CHAPTER 6
MODELS OF PROPOSED INTERMEDIATES FOR THE CATALYZED CYCLIZATION OF ACETYLENES: THE CRYSTAL AND MOLECULAR STRUCTURES OF 1-(π-CYCLOPENTADIENYL)-1-TRIPHENYLPHOSPHINE-2,3,4,5-TETRAKIS(PENTAFLUOROPHENYL)COBALTOLE AND 1-(π-CYCLOPENTADIENYL)-1-TRIPHENYLPHOSPHINE-2,3,4,5-TETRAKIS(PENTAFLUOROPHENYL)RHODOLE

The catalysis of the oligomerization of acetylenes by transition metal complexes has been extensively studied.[90] A reaction mechanism involving a metallo-cyclopentadiene intermediate has been suggested[8-13] for the trimerization of two molecules of acetylene with one of olefin in the presence of $NiBr_2(tpp)_2$, $Ni(CO)_2(tpp)_2$, and other nickel catalysts. Metal-containing hererocycles, metallocycles, have been implicated[14,91-93] as intermediates in the reactions of acetylenes with π-cyclopentadienyldicarbonyl-metal complexes in which the metal was cobalt, rhodium, or iridium. Yamazaki et al.[94-96] on the basis of chemical reactions assigned a metallocyclic structure to a phosphine-containing cobalt complex isolated from the reaction of diphenylacetylene with $Co(cp)(tpp)I_2$ and isopropylmagnesium bromide. They also isolated the same product from the reaction of excess diphenylacetylene with $Co(cp)(tpp)_2$. A preliminary report of the structure of a cobaltacycle formed by the reaction of $Co(cp)(tpp)(PhC{\equiv}CCO_2Me)$ with dimethyl maleate has been reported.[57]

Rausch and Gastinger[15] prepared $C_4(fph)_4Co(cp)(tpp)$ by the reaction of bis(pentafluorophenyl)acetylene with π-cyclopentadienylcarbonyltriphenylphosphinecobalt. The analogous rhodium compound was prepared by the reaction of the corresponding rhodium compound.[15]

Except for one preliminary report[97] no structural data have been available for cobaltacyclopentadiene metallocycles. Therefore, the X-ray diffraction structural analysis of $C_4(fph)_4Co(cp)(tpp)$ was undertaken. The corresponding rhodacycle was studied for comparison with this cobaltacycle and related compounds.

Structure Solution and Refinement for $C_4(fph)_4Co(cp)(tpp)$

The heavy atom method was used in which the positions of the cobalt and phosphorus atoms were estimated from a sharpened Patterson function. A Fourier synthesis based on these atoms was used to estimate the positions of eighteen additional atoms. Successive Fourier syntheses revealed the locations of all nonhydrogen atoms in the compound. A difference Fourier synthesis at that point revealed a region between the cobaltacycles which was of relatively high electron density. Because this density was diffuse no additional atomic positions were estimated before starting refinement, R = 0.27. Three cycles of least-squares refinement with individual isotropic thermal parameters reduced R to 0.14. A difference Fourier synthesis again revealed relatively high elec-

tron density in the same location as before.

Because of the discrepancy of the calculated density ($1.423\ g/cm^3$) from the measured density ($1.59\ g/cm^3$), solvent molecules were presumed to be in the crystal. The deep red crystals of the compound were grown from Skelly C[14] which is a saturated hydrocarbon fraction boiling between 88 and 98°C and consisting mainly of n-heptane, C_7H_{16}. If two solvent molecules were in the unit cell the calculated density would be much nearer the measured value at $1.55\ g/cm^3$. Several maxima were observed in the difference Fourier synthesis within the region of high electron density. The distances between these points and the angles made by lines connecting them did not reasonably approximate a hydrocarbon chain.

The thermal parameters were converted to their anisotropic equivalent and nine least-squares cycles using a block approximation to the matrix reduced R to 0.077. The shifts of all parameters during the final cycle were less than one-tenth of their respective estimated standard deviations. A difference Fourier synthesis calculated at this stage again suggested the presence of an ill-defined solvent molecule. Although the distribution of the peaks, which were not well resolved, suggested a C_7 or C_8 chain, a closer examination of the distances and angles within the group showed them not to reasonably approximate a hydrocarbon chain.

Six peaks were selected which closely retained their positions in the final Fourier summation before refinement and in the difference Fourier syntheses just discussed and

which seemed the most reasonable in approximately a hydrocarbon chain. These locations were used isotropically as carbon atoms together with the seventy-three refined positions from the third full-matrix least-squares cycle used anisotropically in a structure factor calculation and in three cycles of block approximation least-squares refinement. Although almost all the poorly matched reflections ($|F_{obs} - F_{calc}|>20$) improved, a Fourier synthesis revealed peaks at positions shifted to a less reasonable distribution from the linear hydrocarbon approximation used. The refinement was terminated at this point. An outline of the refinement is presented in Table 5.

Scattering factors for cobalt, phosphorus, fluorine, oxygen, and carbon were taken from Hanson et al.[29] A list of observed and calculated structure factors is available.[14]

Structure Solution and Refinement for $C_4(fph)_4Rh(cp)(tpp)$

The method of isomorphous replacement was used for the solution of the structure of $C_4(fph)_4Rh(cp)(tpp)$. The cell constants of $C_4(fph)_4Co(cp)(tpp)$ and $C_4(fph)_4Rh(cp)(tpp)$ as reported in Table 4 are very similar with differences of less than one percent. The positional parameters from the third cycle of full-matrix least-squares refinement for the non-hydrogen atoms in the isomorphous compound $C_4(fph)_4Co(cp)(tpp)$ were used in a structure factor calculation and a difference Fourier synthesis with the $C_4(fph)_4Rh(cp)(tpp)$ data. The structure factor calculation resulted in an R of 0.17 and the

difference Fourier synthesis revealed no major structural differences in the two compounds. The same positional parameters were used in an isotropic least-squares refinement of the $C_4(fph)_4Rh(cp)(tpp)$ data. A summary of further refinement is given in Table 5.

A difference Fourier synthesis after refinement suggested the presence of an ill-defined solvent molecule. As in the case of the cobaltacycle the calculated density, 1.479 g/cm^3, is significantly less than the density of 1.60 g/cm^3 obtained from flotation measurements of the yellow crystals. If two molecules of _n_-heptane are assumed within the unit cell the calculated density would be 1.60 g/cm^3.

An attempt to fit a linear molecule to peaks in the difference Fourier synthesis was also unsuccessful and was not pursued.

The scattering factors used were taken from Hanson _et al._[29] The observed and calculated structures are listed in Table B-5.

Results and Discussion for $C_4(fph)_4Co(cp)(tpp)$ and $C_4(fph)_4Rh(cp)(tpp)$

The final positional and thermal parameters for the nonhydrogen atoms of both $C_4(fph)_4Co(cp)(tpp)$ and $C_4(fph)_4$-$Rh(cp)(tpp)$ are listed in Table 31. The atomic numbering and thermal ellipsoids of the cobaltacycle are shown in Figure 10. The atomic numbering of the rhodacycle is analogous. Selected bond distances and angles for the two compounds are listed

Table 31

Final Atomic Parameters (x 10^4) for the Nonhydrogen Atoms in $C_4(fph)_4Co(cp)(tpp)$ and $C_4(fph)_4$-Rh(cp)(tpp) with Estimated Standard Deviations Given in Parentheses.[a]

Atom	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Co	482(1)	4958(1)	2130(1)	65(1)	64(1)	24(0)	55(2)	32(1)	46(1)
Rh	453(1)	4917(1)	2125(0)	62(1)	63(1)	25(0)	54(1)	29(1)	44(1)
C(1)	1469(8)	4004(8)	2096(5)	78(10)	71(8)	27(3)	70(15)	32(10)	52(9)
	1546(9)	4003(8)	2101(5)	96(11)	71(8)	26(3)	77(16)	36(10)	49(9)
C(2)	2439(8)	4318(8)	1903(5)	89(10)	78(8)	26(3)	95(16)	51(10)	53(9)
	2531(9)	4307(8)	1901(5)	87(10)	61(8)	26(3)	63(15)	41(10)	43(9)
C(3)	2748(8)	5385(7)	1870(5)	72(9)	71(8)	27(3)	84(15)	48(10)	51(9)
	2825(8)	5370(8)	1872(5)	70(9)	68(8)	26(3)	66(15)	34(9)	48(9)
C(4)	1955(8)	5881(7)	2001(5)	78(10)	69(8)	23(3)	52(15)	25(9)	51(9)
	2016(8)	5864(8)	2003(5)	72(9)	75(8)	26(3)	57(15)	27(9)	56(9)
C(11)	1050(9)	2894(8)	2093(5)	88(10)	72(8)	38(4)	80(16)	60(11)	68(10)
	1091(9)	2877(8)	2092(6)	89(11)	73(9)	37(4)	84(16)	52(11)	63(10)
C(12)	1267(9)	2877(8)	2792(6)	89(11)	79(9)	39(4)	76(16)	45(11)	67(10)
	1298(10)	2836(9)	2781(6)	94(11)	89(10)	42(4)	84(17)	55(12)	83(11)
C(13)	889(10)	1830(9)	2778(6)	135(14)	116(11)	51(5)	134(21)	89(14)	117(13)
	902(11)	1800(10)	2759(7)	127(14)	112(11)	56(5)	115(21)	80(14)	117(14)
C(14)	263(12)	754(9)	2043(7)	168(16)	87(10)	68(6)	135(22)	117(17)	107(14)
	273(12)	735(10)	2027(8)	166(16)	83(10)	78(7)	131(22)	122(18)	125(15)
C(15)	19(11)	736(9)	1333(6)	151(15)	80(10)	47(5)	116(20)	97(14)	60(11)
	35(12)	725(9)	1327(7)	147(15)	74(10)	57(6)	81(20)	92(16)	65(13)
C(16)	445(10)	1799(8)	1379(6)	126(13)	80(9)	43(4)	110(18)	87(13)	78(11)
	438(11)	1777(9)	1363(6)	132(13)	82(9)	44(5)	109(19)	84(13)	75(11)

Table 31 - continued

Atom	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
F(12)	1875(6)	3866(5)	3516(3)	148(8)	97(5)	34(2)	91(11)	53(7)	67(6)
	1952(6)	3850(5)	3520(3)	153(8)	98(6)	38(2)	96(11)	54(7)	72(6)
F(13)	1138(7)	1855(6)	3474(4)	215(10)	147(7)	64(3)	164(14)	113(10)	157(9)
	1163(8)	1809(7)	3446(4)	210(11)	160(8)	68(4)	152(16)	101(10)	169(10)
F(14)	-138(8)	-275(6)	2022(5)	272(12)	103(7)	90(4)	182(15)	178(13)	145(9)
	-143(9)	-293(6)	1990(5)	263(13)	100(7)	101(5)	162(16)	158(14)	149(10)
F(15)	-612(7)	-301(5)	622(4)	239(11)	78(6)	65(3)	112(13)	132(10)	62(7)
	-610(9)	-305(6)	602(5)	249(12)	72(6)	70(4)	86(14)	138(12)	52(8)
F(16)	198(6)	1719(5)	670(3)	182(8)	87(5)	37(2)	106(11)	88(8)	54(6)
	188(7)	1725(5)	667(3)	188(9)	86(6)	39(3)	94(12)	79(8)	50(6)
C(21)	3171(9)	3601(8)	1668(5)	106(11)	71(8)	33(4)	87(16)	56(11)	58(10)
	3231(9)	3588(8)	1667(5)	87(10)	74(9)	35(4)	86(16)	51(11)	58(10)
C(22)	4034(10)	3453(9)	2197(6)	123(13)	95(10)	42(4)	135(19)	68(13)	67(11)
	4056(10)	3435(9)	2182(6)	118(13)	86(10)	41(5)	113(19)	60(13)	62(11)
C(23)	4718(12)	2839(11)	1981(7)	145(15)	140(13)	59(6)	190(25)	75(16)	103(15)
	4706(11)	2768(11)	1945(8)	123(14)	114(12)	63(6)	157(22)	67(15)	99(15)
C(24)	4545(12)	2345(11)	1201(8)	154(16)	126(13)	78(7)	198(25)	128(18)	99(16)
	4517(12)	2266(11)	1170(8)	137(15)	113(12)	65(6)	173(23)	98(16)	77(15)
C(25)	3682(11)	2460(9)	647(6)	159(15)	98(11)	48(5)	123(22)	107(15)	58(12)
	3684(12)	2412(10)	635(7)	156(15)	91(11)	45(5)	109(21)	100(15)	50(12)
C(26)	3020(10)	3081(8)	885(6)	112(12)	94(9)	42(4)	103(18)	68(13)	69(11)
	3043(10)	3059(9)	876(6)	100(11)	83(9)	41(4)	95(17)	65(12)	66(11)
F(22)	4250(7)	3923(6)	2967(4)	188(9)	145(7)	47(3)	216(14)	75(8)	100(8)
	4288(7)	3912(6)	2963(4)	170(9)	147(7)	46(3)	204(14)	68(8)	101(8)
F(23)	5532(8)	2681(8)	2501(5)	237(12)	215(10)	81(4)	346(20)	104(12)	152(11)
	5526(9)	2636(8)	2478(5)	228(12)	205(11)	80(4)	337(20)	98(12)	144(12)

Table 31 - continued

Atom	z	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
F(24)	5233(9)	1775(8)	972(5)	261(13)	200(10)	102(5)	359(20)	197(14)	134(12)
	5155(9)	1657(8)	926(6)	233(13)	179(10)	101(5)	310(20)	180(14)	120(12)
F(25)	3500(8)	1971(6)	-124(4)	251(12)	151(8)	65(4)	210(16)	176(11)	97(9)
	3478(8)	1910(7)	-144(4)	238(12)	148(8)	63(4)	200(17)	164(11)	90(9)
F(26)	2165(6)	3179(5)	329(3)	177(9)	111(6)	37(2)	143(12)	79(8)	71(7)
	2223(6)	3177(6)	332(3)	167(9)	118(6)	38(2)	150(13)	77(8)	75(7)
C(31)	3869(9)	5823(7)	1701(5)	92(10)	63(8)	33(4)	77(15)	50(11)	56(9)
	3949(9)	5834(8)	1710(5)	94(11)	68(8)	34(4)	85(16)	51(11)	54(10)
C(32)	3655(9)	5820(8)	992(6)	103(12)	84(9)	37(4)	87(17)	57(12)	61(11)
	3746(10)	5826(9)	1002(6)	108(12)	89(10)	37(4)	91(18)	61(12)	69(11)
C(33)	4687(11)	6121(10)	789(7)	161(15)	119(12)	55(5)	151(22)	135(16)	110(14)
	4764(12)	6138(10)	805(7)	153(15)	106(11)	51(5)	125(22)	114(15)	96(13)
C(34)	5991(11)	6489(10)	1326(7)	113(13)	125(12)	73(6)	123(21)	132(16)	118(15)
	6049(11)	6498(10)	1334(7)	123(13)	112(11)	69(6)	136(21)	144(16)	109(14)
C(35)	6264(9)	6524(9)	2038(7)	80(11)	109(11)	63(6)	108(19)	80(14)	92(13)
	6328(10)	6544(10)	2048(7)	81(11)	100(10)	60(5)	104(18)	73(13)	87(13)
C(36)	5234(9)	6200(9)	2213(6)	104(11)	92(10)	39(4)	111(18)	59(12)	72(11)
	5288(10)	6213(9)	2221(6)	94(11)	90(10)	37(4)	84(18)	42(12)	63(11)
F(32)	2390(6)	5458(5)	454(3)	127(7)	147(7)	43(3)	129(12)	63(7)	107(7)
	2468(6)	5439(6)	459(3)	122(7)	147(7)	40(3)	125(12)	56(7)	104(7)
F(33)	4392(7)	6050(7)	81(4)	225(11)	199(9)	67(4)	212(17)	174(11)	169(10)
	4482(8)	6073(7)	94(4)	212(11)	194(10)	65(4)	204(17)	166(11)	158(10)
F(34)	6973(7)	6763(7)	1127(5)	178(10)	213(10)	111(5)	200(17)	224(13)	206(12)
	7059(8)	6827(8)	1164(6)	164(10)	208(10)	111(5)	198(17)	207(13)	203(13)
F(35)	7531(6)	6879(7)	2557(5)	100(7)	181(9)	93(4)	158(13)	99(9)	154(10)
	7607(6)	6928(7)	2567(5)	88(7)	163(8)	84(4)	127(13)	76(9)	124(10)

Table 31 - continued

Atom	z	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
F(36)	5552(5)	6243(6)	2923(3)	106(7)	157(7)	47(3)	125(12)	48(7)	112(8)
	5597(6)	6265(6)	2930(4)	107(7)	152(7)	46(3)	127(12)	47(7)	105(8)
C(41)	2261(9)	7041(8)	2072(5)	91(10)	75(8)	33(4)	95(16)	64(11)	61(10)
	2290(9)	7009(8)	2054(5)	80(10)	72(8)	32(4)	76(15)	53(10)	59(9)
C(42)	1472(9)	7178(8)	1482(5)	107(11)	90(9)	31(4)	104(18)	50(11)	65(10)
	1474(10)	7113(9)	1470(6)	98(11)	83(9)	34(4)	88(17)	45(11)	67(10)
C(43)	1764(10)	8273(9)	1579(6)	137(14)	109(11)	49(5)	150(21)	81(14)	109(13)
	1711(12)	8169(10)	1549(7)	150(15)	118(12)	50(5)	157(22)	84(15)	115(14)
C(44)	2816(11)	9268(9)	2269(7)	143(14)	79(9)	61(6)	110(20)	106(15)	95(13)
	2786(12)	9217(10)	2252(7)	144(14)	91(11)	68(6)	128(21)	111(16)	113(14)
C(45)	3644(10)	9168(8)	2845(6)	105(12)	79(9)	45(5)	54(18)	70(13)	57(11)
	3630(10)	9135(9)	2818(6)	103(12)	84(10)	45(5)	51(18)	64(13)	54(11)
C(46)	3377(8)	8066(8)	2729(5)	78(10)	68(8)	32(4)	54(15)	39(10)	52(9)
	3405(9)	8064(8)	2722(6)	94(11)	73(9)	37(4)	72(16)	56(11)	65(10)
F(42)	388(5)	6210(5)	778(3)	129(7)	110(6)	35(2)	99(11)	34(7)	78(6)
	402(6)	6129(5)	785(3)	127(7)	107(6)	38(2)	96(11)	30(7)	78(6)
F(43)	970(7)	8332(6)	986(4)	213(10)	152(8)	74(4)	214(15)	100(10)	166(9)
	887(8)	8225(7)	964(5)	198(11)	165(9)	79(4)	204(16)	92(11)	179(10)
F(44)	3063(8)	10324(6)	2369(5)	236(11)	96(6)	93(4)	155(14)	133(12)	131(9)
	3005(8)	10263(6)	2332(5)	236(12)	98(7)	100(5)	172(15)	144(13)	137(10)
F(45)	4746(6)	10156(5)	3532(4)	162(9)	81(6)	61(3)	35(11)	75(9)	55(7)
	4715(7)	10148(5)	3495(4)	164(9)	73(6)	64(3)	31(12)	79(9)	47(7)
F(46)	4247(5)	8032(5)	3315(3)	100(6)	94(5)	38(2)	68(10)	34(6)	63(6)
	4296(5)	8055(5)	3305(3)	100(6)	93(5)	37(2)	64(10)	29(6)	59(6)
C(51)	-1476(9)	4842(10)	1969(6)	63(10)	125(11)	40(4)	70(18)	22(11)	77(12)
	-1641(9)	4744(11)	1924(6)	63(10)	133(13)	43(5)	72(19)	27(12)	77(13)

Table 3.1 - continued

Atom	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
C(52)	-1486(9)	3709(9)	1766(6)	64(10)	112(11)	50(5)	26(18)	25(12)	90(13)
	-1672(10)	3638(11)	1750(7)	66(11)	125(13)	56(6)	6(19)	16(13)	103(14)
C(53)	-1196(10)	3326(9)	1116(6)	99(12)	84(10)	34(4)	61(18)	10(12)	41(11)
	-1403(10)	3198(10)	1083(7)	77(11)	90(10)	48(5)	29(18)	1(12)	54(12)
C(54)	-929(9)	4195(8)	911(5)	88(11)	89(9)	29(4)	81(17)	21(11)	40(10)
	-1161(10)	4034(10)	847(6)	81(11)	108(11)	30(4)	73(18)	10(11)	41(11)
C(55)	-1115(9)	5132(9)	1426(6)	77(11)	111(10)	35(4)	80(18)	19(11)	73(11)
	-1339(9)	4970(10)	1355(6)	71(10)	104(11)	41(4)	62(17)	16(11)	69(12)
P	1381(2)	6265(2)	3462(1)	72(3)	71(2)	26(1)	61(4)	39(3)	52(2)
	1433(2)	6288(2)	3493(1)	71(3)	72(2)	26(1)	62(4)	38(3)	53(2)
C(60)	174(9)	5972(8)	3855(5)	77(10)	97(10)	30(4)	67(16)	44(10)	61(10)
	188(9)	5980(9)	3869(6)	82(10)	108(10)	30(4)	75(17)	52(11)	71(11)
C(61)	-309(10)	4875(10)	3800(6)	118(13)	117(11)	53(5)	95(20)	87(14)	109(13)
	-282(11)	4899(10)	3822(7)	126(14)	123(12)	50(5)	99(22)	88(14)	111(14)
C(62)	-1268(12)	4596(11)	4068(8)	143(15)	158(15)	66(6)	103(25)	119(17)	140(17)
	-1248(13)	4597(12)	4062(8)	162(17)	146(15)	67(7)	124(26)	124(18)	130(17)
C(63)	-1740(12)	5396(12)	4382(8)	160(17)	160(15)	65(6)	126(26)	134(18)	121(17)
	-1735(14)	5371(14)	4357(9)	159(18)	171(17)	74(7)	132(29)	136(20)	137(19)
C(64)	-1260(14)	6475(12)	4438(8)	206(20)	158(16)	80(8)	182(30)	202(22)	129(19)
	-1248(15)	6446(14)	4401(10)	188(20)	184(18)	91(9)	213(33)	196(23)	156(22)
C(65)	-281(11)	6770(10)	4179(7)	156(15)	130(12)	59(6)	161(23)	140(16)	105(14)
	-311(12)	6748(11)	4152(7)	135(15)	137(13)	60(6)	147(24)	128(16)	99(15)
C(70)	2931(9)	6458(8)	4204(5)	93(11)	67(8)	30(4)	53(16)	30(11)	53(10)
	2953(9)	6484(8)	4230(5)	73(10)	72(8)	29(4)	60(15)	26(10)	53(9)
C(71)	3110(10)	6734(9)	4984(6)	130(13)	96(10)	33(4)	76(19)	47(12)	72(11)
	3141(11)	6760(10)	5001(6)	111(13)	118(12)	35(4)	70(20)	36(12)	81(12)

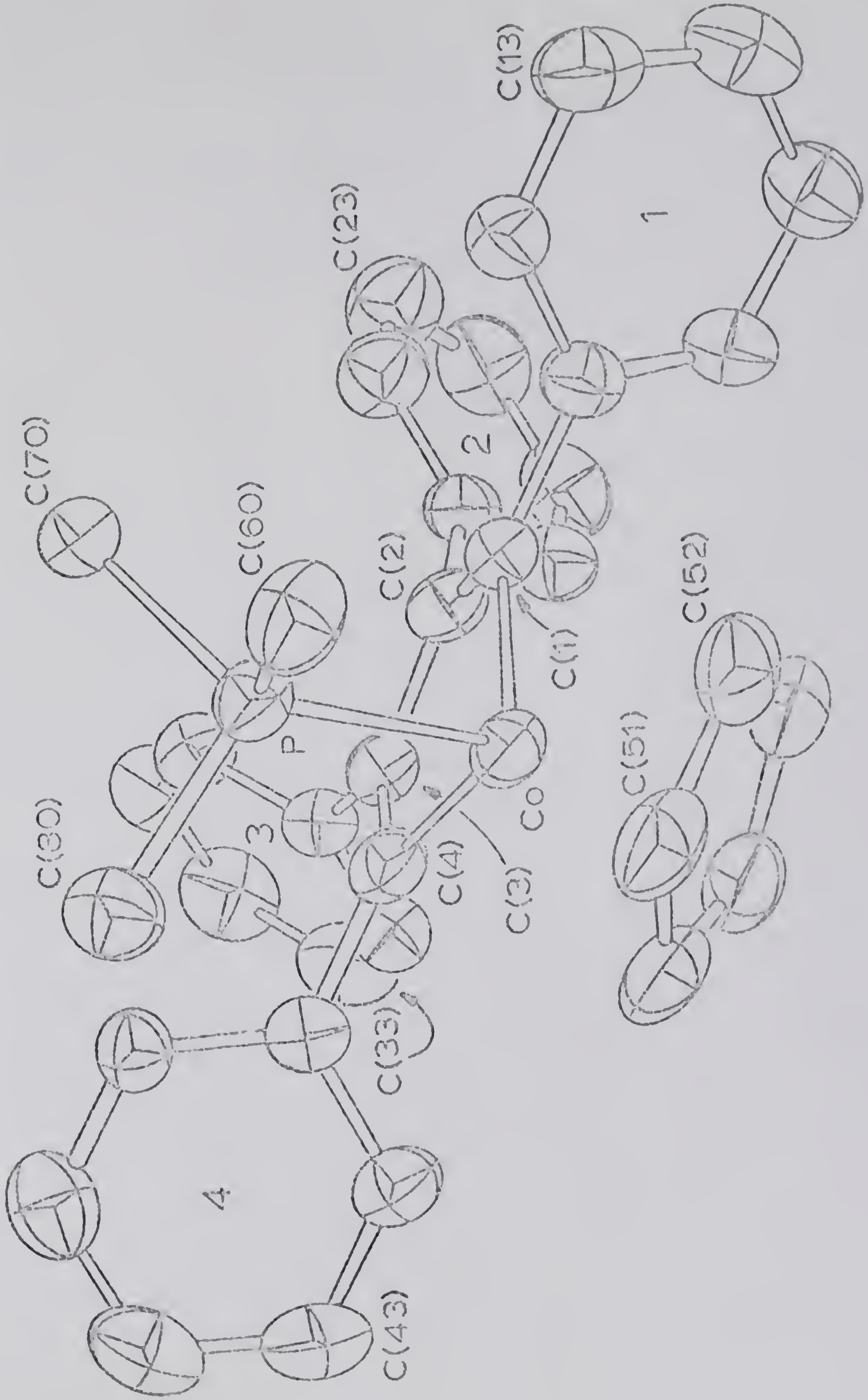
Table 31 - continued

Atom	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
C(72)	4288(11)	6884(10)	5544(6)	121(14)	122(12)	42(5)	56(21)	24(13)	92(13)
	4315(12)	6902(12)	5555(7)	123(14)	145(14)	42(5)	77(23)	26(14)	102(14)
C(73)	5256(11)	6731(10)	5313(7)	113(14)	128(13)	54(5)	81(22)	22(14)	102(14)
	5271(12)	6770(11)	5344(7)	116(14)	130(13)	52(6)	84(23)	25(14)	101(15)
C(74)	5079(10)	6465(10)	4545(6)	102(13)	116(12)	46(5)	92(20)	27(13)	74(13)
	5119(11)	6504(11)	4572(7)	109(14)	118(13)	52(6)	81(22)	20(14)	78(14)
C(75)	3935(9)	6342(8)	3993(6)	76(10)	85(9)	38(4)	72(16)	32(11)	58(10)
	3938(9)	6368(9)	4025(6)	79(11)	91(10)	37(4)	72(17)	22(11)	59(11)
C(80)	1783(9)	7786(8)	3738(5)	101(11)	77(9)	31(4)	84(16)	66(11)	58(10)
	1836(9)	7791(8)	3744(5)	91(11)	85(9)	32(4)	90(16)	56(11)	66(10)
C(81)	857(9)	7958(8)	3226(6)	109(12)	93(10)	41(4)	115(18)	77(12)	76(11)
	938(10)	7945(9)	3225(6)	117(13)	91(10)	37(4)	109(19)	65(12)	67(11)
C(82)	1115(11)	9122(10)	3440(7)	144(14)	112(11)	54(5)	154(21)	107(15)	100(13)
	1146(12)	9094(10)	3420(7)	150(15)	91(10)	53(5)	135(21)	94(15)	89(13)
C(83)	2298(11)	10114(10)	4154(7)	143(15)	99(11)	58(6)	109(21)	103(16)	81(13)
	2317(13)	10102(10)	4129(8)	158(16)	98(11)	53(6)	115(23)	101(17)	76(14)
C(84)	3216(11)	9918(9)	4656(7)	117(14)	84(10)	53(5)	80(20)	81(15)	69(12)
	3211(12)	9921(10)	4638(7)	133(15)	91(11)	55(6)	85(21)	67(15)	70(13)
C(85)	2968(10)	8774(9)	4448(6)	113(12)	83(10)	38(4)	65(18)	53(12)	58(11)
	2980(10)	8797(9)	4458(6)	105(12)	81(10)	42(5)	69(18)	54(12)	57(11)

[a]The coordinates of the atoms in each structure are listed in order of the metal atom.

Figure 10

An ORTEP drawing of $C_4(fph)_4Co(cp)(tpp)$ showing the atomic numbering and thermal ellipsoids. The fph rings are numbered 1-4 and the fluorines have been omitted for clarity. Similarly, the three phenyl rings of the tpp ligand have been omitted with only the first atoms C(60), C(70), and C(80) shown.


C(13)
C(23)
1
C(70)
C(60)
C(2)
2
C(52)
C(1)
C(51)
P
Co
C(30)
3
C(4)
C(3)
C(33)
4
C(43)

in Tables 32 and 33. Least-squares planes and deviations are given in Table 34.

The molecules are metallocycles with the metal atom also bonded to the cyclopentadienyl ring and to the triphenylphosphine ligand. The C(1) to C(4) fragment in both compounds is planar with the largest deviation from the best plane being 0.015 Å in the cobalt compound and 0.017 Å in the rhodium compound. The metal atoms, however, are significantly displaced from the plane in the direction of the cp ring by -0.203 and -0.239 Å. This perpendicular displacement is similar to that found in other similar metallocycles.[98]

The metallocycles may be considered as a delocalized diene with the metal atom σ-bonded to the two carbon atoms of the ring, C(1) and C(4). The Co-C bond distances, 1.995 (11) and 1.993(11) Å, and the Rh-C bond distances, 2.060(12) and 2.067(11) Å, are similar to various values given by Churchill.[99] Values of 1.979(1) Å[48] and 1.990(5) Å[51] have more recently been reported for Co-C bonds in cobaloxime complexes. Mague[100,101] has reported structures of similar rhodacyles in which the Rh-C distances are 2.000(11), 1.964 (11), 2.047(16), and 1.998(16) Å. Also, Cotton and Norman[102] report a single-bond covalent radius of 1.39 Å for Rh(III). When this value is added to half the 1.485 Å suggested length for a single-bond between sp^2 carbon atoms[103] the Rh-C distance is predicted to be 2.13 Å. The observed Rh-C distances where rhodium has a formal oxidation number of +1 are shorter than the above predicted single-bond distance. This differ-

Table 32
Selected Bond Distances (Å) of $C_4(fph)_4M(cp)(tpp)$ (M=Co,Rh) with Their Estimated Standard Deviations in Parentheses.

M =	Co	Rh
M - C(1)	1.995(11)	2.060(12)
M - C(4)	1.993(11)	2.067(11)
M - P	2.234(3)	2.293(2)
M - C(51)	2.157(12)	2.286(13)
M - C(52)	2.121(13)	2.261(14)
M - C(53)	2.119(11)	2.250(13)
M - C(54)	2.104(9)	2.238(10)
M - C(55)	2.133(12)	2.268(12)
C(1)-C(2)	1.326(15)	1.343(16)
C(2)-C(3)	1.467(16)	1.457(16)
C(3)-C(4)	1.335(15)	1.354(15)
C(1)-C(11)	1.487(16)	1.498(17)
C(2)-C(21)	1.523(16)	1.497(16)
C(3)-C(31)	1.481(15)	1.478(16)
C(4)-C(41)	1.493(16)	1.492(17)
P-C(60)	1.848(11)	1.858(12)
P-C(70)	1.843(11)	1.821(10)
P-C(80)	1.834(12)	1.820(13)
C(51)-C(52)	1.463(20)	1.429(22)
C(52)-C(53)	1.400(16)	1.420(17)
C(53)-C(54)	1.426(18)	1.424(20)
C(54)-C(55)	1.433(16)	1.422(17)
C(55)-C(51)	1.457(17)	1.431(18)

Table 33

Selected Bond Angles (°) of $C_4(fph)_4M(cp)(tpp)$ with Their Estimated Standard Deviations Given in Parentheses. (M=Co,Rh)

M =	Co	Rh
M-C(1)-C(2)	112.1(8)	115.5(8)
C(1)-C(2)-C(3)	116.8(9)	114.9(9)
C(2)-C(3)-C(4)	114.8(9)	115.5(9)
M-C(4)-C(3)	113.1(7)	114.8(8)
C(1)-M-C(4)	82.4(4)	78.3(4)
P-M-C(1)	103.0(3)	101.6(3)
P-M-C(4)	95.2(3)	93.3(3)
C(11)-C(1)-M	127.0(7)	123.3(8)
C(11)-C(1)-C(2)	119.6(9)	119.4(10)
C(21)-C(2)-C(1)	123.9(9)	124.1(10)
C(21)-C(2)-C(3)	119.2(9)	120.9(9)
C(31)-C(3)-C(2)	119.7(9)	119.7(9)
C(31)-C(3)-C(4)	125.5(9)	124.9(10)
C(41)-C(4)-C(3)	119.8(9)	120.3(9)
C(41)-C(4)-M	127.0(7)	124.9(7)
C(51)-C(52)-C(53)	108.1(11)	108.3(12)
C(52)-C(53)-C(54)	109.8(10)	108.8(11)
C(53)-C(54)-C(55)	107.7(10)	106.9(11)
C(54)-C(55)-C(51)	108.0(10)	109.3(11)
C(55)-C(51)-C(52)	106.3(10)	106.8(11)

Table 34

Deviations from and Equations of Some Lease-Squares Planes of $C_4(fph)_4Co(cp)(tpp)$ and $C_4(fph)_4Rh(cp)(tpp)$.[a]

(a) Deviations (Å x 10^{+3})

Atom	Plane 1	Plane 2	Plane 3	Plane 4
Co	-203		1741	
Rh		-239		1908
C(1)	8*	9*		
C(2)	-15*	-17*		
C(3)	14*	17*		
C(4)	-8*	-9*		
C(51)	-931	-1058	-7*	2*
C(52)	-1211	-1307	15*	6*
C(53)	-2043	-2168	-16*	-12*
C(54)	-2265	-2437	11*	13*
C(55)	-1598	-1774	-2*	-9*
P	1884	1922	3025	3241

(b) Coefficients of the Plane[59] AX + BY + CZ = D

Plane	A	B	C	D
1	0.2201	0.0627	0.9735	3.2807
2	0.2193	0.0672	0.9733	3.3160
3	0.7356	0.1345	0.6639	-0.8420
4	0.7474	0.1591	0.6450	-1.0481

[a]The entries marked with an asterisk were used to define the plane.

ence could be indicative of multiple bonding between the terminal carbon atoms of the diene and the metal atom. The C-C distances in the metallocycle rings fall into two groups. The C(1)-C(2) and C(3)-C(4) distances are equal within experimental error to the accepted value of 1.337(6) Å for a simple C-C double bond.[104] The C(2)-C(3) distances are indicative of a C-C single bond between two double bonds.[104] The observations of Mague[100,101] on two rhodacycles suggested a double-bond system similar to those in $C_4(fph)_4Co(cp)(tpp)$ and $C_4(fph)_4Rh(cp)(tpp)$.

The cp rings in the compounds are planar with the maximum deviations from the least-squares planes of -0.016 and -0.012 Å. The distances from the cp ring atoms to the metal atom show that the metal atom is slightly displaced from the center of the cp ring. The range of the Co-C(cp ring) distances is from 2.104(9) to 2.157(12) Å with a mean of 2.127 (9) Å. These values are similar to those in other Co-cp complexes.[105,106]

In both the cobalt and rhodium compounds the longest metal-C(cp ring) distance involves C(51), the carbon atom nearest the phosphine ligand. The mean Rh-C(cp ring) distance is 2.286(13) Å. This value is equivalent to the mean distance of 2.246(9) Å in $Rh(C_2F_5)(cp)I(CO)$[107] and falls within the 2.19 to 2.26 Å range reported for corresponding mean values for other cp-rhodium complexes.[108]

The C-C bond distances within the cp rings range from 1.400(16) to 1.463(20) Å with a mean of 1.436(11) Å in the

cobalt compound and a range from 1.420(17) to 1.431(18) Å with a mean of 1.425 Å in the rhodium compound. These C-C distances are comparable to those found in other cp complexes.[105,106,109] The cp rings are tipped relative to the C(1) to C(4) planes by 35.3° and 36.6°.

The Co-P distance of 2.234(3) Å is similar to the Co-P distance in five-coordinate complexes of cobalt where the range is reported[110] to be from 2.192(6) to 2.27(1) Å. Also, in cobalt-carbonyl complexes such as $Co_4(CO)_{10}(Ph_2PC{\equiv}CCF_3)_2$ and $Co(CO)_2(NO)(tpp)$ the Co-P distances are 2.236 and 2.229 Å[111] in the former and 2.224(3) and 2.230(3) Å[112] in the latter. The Rh-P distance of 2.293(3) Å is similar to those in phosphine complexes of rhodium(I).[113] The metal to phosphine distance in metal-oxime complexes have been found to be somewhat longer.[40,97] The Co-P distance in cobaloxime complexes has been reported as 2.327(4) Å[40] and 2.339(1) Å.[48] The Rh-P distance in $RhC\ell(Hdmg)_2(tpp)$ was reported to be 2.327(1) Å.[102] Since the distances in oxime complexes in both cobalt and rhodium are equivalent, the phosphorus atom may be in the position of closest approach to the metal atom as limited by the steric constraints of the oxime ligands.

The distances in the fph rings have been summarized in Table 35. The individual values for the distances and angles in the fph rings on the metallocycles and the phenyl rings of the phosphines are given in Tables 36-38. The dimensions are not unusual and are in agreement with expected values.

Table 35

Average C-F and C-C Distances for the Pentafluorophenyl Groups in $C_4(fph)_4M(cp)(tpp)$ with Estimated Standard Deviations[a] Given in Parentheses (M=Co,Rh).

	(a) C-F Distances (Å)		(b) C-C Distances (Å)	
M =	Co	Rh	Co	Rh
All Rings	1.344(2)	1.344(2)	1.378(3)	1.373(3)
Ring 1	1.342(6)	1.340(3)	1.385(1)	1.376(4)
Ring 2	1.345(4)	1.347(4)	1.373(4)	1.371(9)
Ring 3	1.340(3)	1.345(3)	1.384(8)	1.375(6)
Ring 4	1.348(4)	1.346(3)	1.372(8)	1.371(7)

[a] Standard deviations were estimated using the equation:

$$\sigma = \left[\sum_{i=1}^{n}(x_i-\bar{x})^2/N(N-1)\right]^{1/2}$$

Table 36
Bond Distances and Bond Angles of Pentafluorophenyl Groups in $C_4(fph)_4Rh(cp)(tpp)$.

(a) Distances (Å)

n =	1	2	3	4
Cn1-Cn2	1.384(15)	1.342(16)	1.392(15)	1.385(15)
Cn2-Cn3	1.364(20)	1.400(20)	1.374(20)	1.351(20)
Cn3-Cn4	1.375(18)	1.358(18)	1.357(19)	1.389(18)
Cn4-Cn5	1.367(19)	1.365(20)	1.368(18)	1.355(19)
Cn5-Cn6	1.372(20)	1.373(19)	1.367(18)	1.362(19)
Cn6-Cn1	1.393(15)	1.389(14)	1.389(16)	1.386(14)
Cn2-Fn2	1.347(12)	1.354(12)	1.351(13)	1.344(12)
Cn3-Fn3	1.339(15)	1.341(18)	1.349(15)	1.348(16)
Cn4-Fn4	1.338(18)	1.337(19)	1.335(18)	1.340(18)
Cn5-Fn5	1.343(15)	1.358(14)	1.338(15)	1.357(14)
Cn6-Fn6	1.331(13)	1.343(14)	1.351(13)	1.342(13)

(b) Angles (°)

Cn1-Cn2-Cn3	123.1(11)	122.4(12)	123.7(11)	122.9(11)
Cn2-Cn3-Cn4	119.6(13)	119.3(13)	118.8(13)	120.2(13)
Cn3-Cn4-Cn5	119.6(13)	119.3(14)	120.8(13)	117.9(13)
Cn4-Cn5-Cn6	119.8(13)	120.6(13)	119.0(12)	121.4(12)
Cn5-Cn6-Cn1	122.6(12)	121.1(11)	123.6(11)	122.0(11)
Cn6-Cn1-Cn2	115.3(11)	117.3(11)	114.1(10)	115.4(10)
Cn -Cn1-Cn2	124.2(10)	123.9(10)	123.1(10)	124.1(10)
Cn -Cn1-Cn6	120.5(10)	118.8(10)	122.5(10)	120.5(10)
Fn2-Cn2-Cn1	120.2(10)	121.3(11)	118.2(10)	119.4(10)
Fn2-Cn2-Cn3	116.7(11)	116.4(11)	118.0(11)	117.7(11)
Fn3-Cn3-Cn2	120.9(12)	120.7(13)	120.3(12)	120.8(12)
Fn3-Cn3-Cn4	119.5(12)	120.0(13)	120.9(12)	119.0(12)
Fn4-Cn4-Cn3	120.7(13)	121.3(14)	119.9(13)	119.9(12)
Fn4-Cn4-Cn5	119.7(13)	119.4(13)	119.3(13)	122.1(13)
Fn5-Cn5-Cn4	120.9(13)	120.1(13)	119.6(12)	118.8(12)

Table 36 - continued

n =	1	2	3	4
Fn6-Cn6-Cn5	115.7(10)	118.3(11)	117.6(10)	117.2(9)
Fn6-Cn6-Cn1	120.4(10)	118.8(10)	118.5(10)	119.7(9)

Table 37
Bond Distances and Bond Angles of Pentafluorophenyl Groups in $C_4(fph)_4Co(cp)(tpp)$.

(a) Distances (Å)

n =	1	2	3	4
Cn1-Cn2	1.387(14)	1.372(16)	1.394(14)	1.403(15)
Cn2-Cn3	1.388(19)	1.368(20)	1.398(19)	1.358(19)
Cn3-Cn4	1.387(17)	1.374(18)	1.370(18)	1.348(16)
Cn4-Cn5	1.382(17)	1.374(20)	1.372(18)	1.370(17)
Cn5-Cn6	1.382(18)	1.363(19)	1.362(18)	1.384(17)
Cn6-Cn1	1.385(14)	1.389(14)	1.408(15)	1.367(14)
Cn2-Fn2	1.322(11)	1.341(12)	1.339(13)	1.358(11)
Cn3-Fn3	1.350(14)	1.338(17)	1.339(14)	1.338(14)
Cn4-Fn4	1.360(17)	1.339(19)	1.334(17)	1.335(16)
Cn5-Fn5	1.336(13)	1.354(13)	1.330(14)	1.361(13)
Cn6-Fn6	1.341(12)	1.355(13)	1.356(12)	1.348(12)

(b) Angles (°)

	1	2	3	4
Cn1-Cn2-Cn3	122.4(11)	122.9(12)	123.4(11)	122.6(10)
Cn2-Cn3-Cn4	119.7(12)	119.2(13)	118.9(12)	120.5(12)
Cn3-Cn4-Cn5	119.6(12)	120.1(14)	120.2(13)	118.7(12)
Cn4-Cn5-Cn6	118.7(12)	119.0(12)	119.8(12)	120.4(11)
Cn5-Cn6-Cn1	123.9(11)	122.9(11)	123.8(11)	123.0(10)
Cn6-Cn1-Cn2	115.6(10)	116.0(10)	113.9(10)	114.5(10)
Cn -Cn1-Cn2	123.3(10)	123.8(10)	122.9(9)	124.2(9)
Cn -Cn1-Cn6	121.0(10)	120.2(10)	123.0(9)	121.3(9)
Fn2-Cn2-Cn1	121.4(10)	120.5(10)	119.1(10)	119.8(9)
Fn2-Cn2-Cn3	116.2(10)	116.6(11)	117.5(10)	117.7(10)
Fn3-Cn3-Cn3	120.4(11)	122.0(13)	119.9(11)	119.1(11)
Fn3-Cn3-Cn4	119.9(11)	118.8(13)	121.2(12)	120.4(11)
Fn4-Cn4-Cn3	120.0(12)	121.2(13)	118.9(12)	120.1(11)
Fn4-Cn4-Cn5	120.4(12)	118.7(13)	120.9(12)	121.2(11)
Fn5-Cn5-Cn4	119.7(11)	120.5(12)	119.9(12)	119.8(11)
Fn5-Cn5-Cn6	121.6(11)	120.5(12)	120.3(11)	119.8(10)

Table 37 - continued

n =	1	2	3	4
Fn5-Cn5-Cn6	119.4(12)	119.3(12)	121.4(12)	119.8(11)
Fn6-Cn6-Cn5	117.7(11)	119.0(11)	117.6(11)	117.9(10)
Fn6-Cn6-Cn1	119.7(11)	119.9(10)	118.9(10)	120.1(10)

Table 38

Bond Distances and Bond Angles of Triphenylphosphine in $C_4(fph)_4M(cp)(tpp)$.

(a) Distances (Å)

	n = 6		7		8	
M =	Co	Rh	Co	Rh	Co	Rh
P-C(n0)	1.848(11)	1.858(12)	1.843(11)	1.821(10)	1.834(12)	1.820(13)
C(n0)-C(n1)	1.419(19)	1.400(20)	1.411(14)	1.387(14)	1.416(16)	1.395(16)
C(n1)-C(n2)	1.414(20)	1.382(22)	1.394(17)	1.399(19)	1.413(19)	1.413(20)
C(n2)-C(n3)	1.397(22)	1.379(25)	1.386(19)	1.347(21)	1.416(17)	1.413(19)
C(n3)-C(n4)	1.394(25)	1.396(30)	1.390(17)	1.405(18)	1.422(19)	1.406(21)
C(n4)-C(n5)	1.423(23)	1.367(25)	1.376(16)	1.403(18)	1.391(19)	1.380(21)
C(n5)-C(n0)	1.387(18)	1.377(20)	1.394(16)	1.368(16)	1.413(14)	1.404(15)

(b) Angles (°)

	n = 6		7		8	
M =	Co	Rh	Co	Rh	Co	Rh
P-C(n0)-C(n1)	117.7(8)	117.4(9)	120.3(8)	121.4(9)	118.3(8)	118.5(9)
P-C(n0)-C(n5)	122.2(9)	122.2(10)	119.6(8)	119.5(8)	121.8(8)	122.3(9)
C(n0)-C(n1)-C(n2)	119.7(12)	120.1(13)	119.9(11)	120.3(12)	119.5(11)	121.0(11)
C(n1)-C(n2)-C(n3)	120.0(13)	119.7(15)	119.0(12)	120.3(14)	120.7(12)	119.5(12)
C(n2)-C(n3)-C(n4)	120.2(14)	119.2(16)	120.8(13)	120.8(14)	118.7(12)	118.2(13)
C(n3)-C(n4)-C(n5)	120.2(14)	121.8(17)	120.8(12)	118.2(13)	120.8(12)	122.0(13)
C(n4)-C(n5)-C(n0)	119.8(13)	118.8(14)	119.2(11)	121.3(11)	120.3(11)	120.1(12)
C(n5)-C(n0)-C(n1)	120.0(11)	120.4(12)	120.1(10)	119.1(11)	119.9(10)	119.1(11)

Table 38 - continued

	M = Co	Rh
C(60)-P-C(70)	102.7(5)	103.5(5)
C(60)-P-C(80)	100.9(5)	101.8(5)
C(70)-P-C(80)	103.0(5)	103.8(5)

The fluorinated metallocycles resist thermal decomposition better than the hydrocarbon analogs.[14,15] Enhanced thermal stabilities have been observed in other highly fluorinated metallocycles relative to their hydrocarbon analogs.[114] In the compounds of this study the triphenylphosphine ligand and the four fph rings provide an effective shield for the two double bonds in the metallocycles. Although the fluorine atoms of the fph rings and the phenyl rings of the tpp were omitted from Figure 10, the sterically hindered nature of the metallocycle may easily be seen. The lack of a convenient path for an attacking acetylene together with the enhanced thermal stability of the fluorinated derivatives may have allowed the isolation of these intermediate metallocycles. Metallocycles of cobalt and rhodium of the type presented are reasonable intermediates in the catalyzed oligomerization of acetylenes.

CHAPTER 7
CONCLUDING REMARKS

The structure of $C\ell Co(H_2dmg)(dmg)(clan)$ shows the same LIPS phenomenon as $C\ell Co(H_2dmg)(dmg)(sulfa)$.[46] These two compounds exhibit the unusual feature of containing both neutral and dianionic dimethylglyoxime groups. Also, the orientation of the benzene ring of the sulfa and clan group in the respective compounds is over the dianionic dmg. The various distances and the relative orientation of the axial ligand in both compounds suggest a π-type interaction. LIPS supports the contention that "hydrophobic forces" are important in enzymic processes.[3] The bis(diglyoximato)cobalt(III) complexes of aniline derivatives have here been shown to be useful models for the examination of this type interaction. An extension of X-ray structural determinations to similar compounds with other aniline derivatives and with other diglyoximes is suggested. Low-temperature X-ray studies could effect better resolution of the inter-dmg bridge structure and the N-O distances.

An investigation of the fluorescence spectra of these compounds could reveal additional information concerning the interaction between the equatorial and axial ligands. The fluorescence of 5-dimethylaminonaphthalene-1-sulfonamide was observed to be enhanced while the fluorescence of carbonic

anhydrase was diminished when a 1:1 complex of the two was formed.[51] Although the major contribution to this observation is believed to be the ionization of the sulfonamide, a portion of the change is attributed to a hydrophobic interaction.[51,115] The fluorescence spectra of cobaloxime complexes with aniline derivatives should help reveal the nature of the interligand interaction as a function of the orientation angle.

The novel ligand dhphpy has been demonstrated as a binucleating ligand. The bridging site occupied by a chlorine atom in $[Ni_2C\ell(H_2O)_4(dhphpy)]C\ell_3$ clearly is accessible and of convenient dimensions to accommodate a molecule such as dinitrogen. Further development of this system as a possible model for nitrogenase should include use of molybdenum salts and work with the exclusion of oxygen. Synthesis of similar ligands with saturated "side arms" is also suggested.

The compounds $C_4(fph)_4Co(cp)(tpp)$ and $C_4(fph)_4Rh(cp)(tpp)$ contain a butadiene fragment with each end bound to a metal atom. The metal to carbon bonds are shorter than expected for the single-bonded distance. The metallocycles are, therefore, believed to contain a delocalized π-bonding system. While metallocycles should be highly susceptible to nucleophilic attack and thermal decomposition the two compounds studied here are very stable. The enhancement of thermal stability by the fluorinated substituents may be at least partially responsible. Also, the presence of the four fph rings

along with the tpp and cp ligands provides a shield from attack for the metallocycle.

The understanding of catalytic processes should improve the efficiency of our existence. Hopefully, enzymic processes occurring in nature can be duplicated in the laboratory by suitable models. These model enzyme systems may then be applied to cure the diseased and feed the hungry.

APPENDIX A
BOOTHIT1

A listing of the FORTRAN language computer program BOOTHIT1 follows. This program was designed to interpolate atomic positional parameters by Booth's method[116] from the values of a Fourier synthesis calculation. The Fourier synthesis program written by Dr. Gus J. Palenik was modified to store the calculated values on a magnetic disk. After supplying BOOTHIT1 with input data of the approximate position of each atom, the stored values are retrieved. The program estimates the position of maximum electron density for each atom from these Fourier synthesis values. The positional parameters may be translated to equivalent positions and may be passed to a bond distance and angle program. The resulting fractional coordinates are punched into IBM cards in the format required for their input into the Fourier synthesis and least-squares refinement programs.

```
C * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
C
C
C                                 BOOTHIT1
C
C
C * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
C
C
C    THIS IS A PROGRAM TO BOOTH VALUES FOR ATOMIC POSITIONS DIRECTLY
C    FROM FOURIER CALCULATIONS STORED ON DISK
C
C
C * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
C
C
C    SUMMARY OF INPUT CARDS FOLLOWS
C
C     CARD 1. TITLE
C
C     CARD 2.   NFO; NABR, IF, IS, IT, ISEL, ICENT, NMOD, IDUMP AS IN
C       FOURIER, THEN ATMPAS.  IF ATMPAS IS GREATER THAN ZERO, THE
C       ATOMIC PARAMETERS WILL BE WRITTEN ONTO UNIT 04 TO BE PASSED ON
C       TO THE BOND ANGLES PROGRAM.  THEY WILL BE IN THE SAME ORDER
C       AS THEY WERE READ.
C
C     CARD(S) 3. EQUIVALENT POSITIONS CARDS. (MAY NEED MORE FOR
C       TRANSLATIONS THAN WERE NEEDED FOR FOURIER.)
C
C     CARD 4. NV, NU, IORGN FOR H, K, &L FOLLOWED BY NATOMS AND IDISK
C       WHERE IDISK IS THE UNIT ON WHICH THE FOURIER IS STORED,
C       THE NORMAL ORIGIN IS -1, -1, -1.
C
C     CARD(S) 5. FORMAT(6I4, 6F8.5, I2, I3, A3)
C       IPIC(X),(Y),&(Z) ARE THE DIVISIONAL COORDINATES, NTRX, NTRY, AND
```

```
C         NTRZ ARE ANY DESIRED UNIT TRANSLATIONS. B'S AND LFT FOLLOW.
C         IPIC VALUES SHOULD BE LESS THAN NV.
C
C         IT IS BETTER TO ESTIMATE IPIC(I) WHERE I IS THE LAST SUMMED
C         INDEX A LOWER VALUE THAN A HIGHER VALUE SINCE THE PROGRAM IS
C         SEARCHING ONLY THREE SECTIONS AT A TIME
C
C         NREQ IS THE EQUIVALENT POSITION CARD NO.  IF NREC IS NEGATIVE
C         POSITIONAL COORDINATES ARE * -1.
C         TRANSLATIONS PERFORMED BY THIS PROGRAM WILL NOT INTERCHANGE
C         X, Y, OR Z.
C
C * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
C
C                                                   DOUG SULLIVAN  OCT. 1974
C
C
      DIMENSION IPIC(99,03), PFS1(60,120), PFS2(60,120), PFS3(60,120),
     1 NTRX(99), NTRY(99), NTRZ(99), B11(99), B22(99), B33(99), B12(99),
     2 B13(99), B23(99), LFT(99), NREQ(99), CODW(99), PTW(12,08),
     3 IDENT(6,8),  IORGN(3), NU(3), NV(3), IU(99), IV(99), IW(99),
     4 FC(99,3), TMAX(99), X(99), Y(99), Z(99), ITITLE(20)
      COMMON IPIC,NATS,IF,IS,IT,IVF,IVS,IVT,TMAX,IU,IV,IW,PFS1,PFS2,
     1 PFS3, NF,NS,NT,FC,MLEVEL,NVS,NVF,CODW
   01 FORMAT(6I4,6F8.5,I2,I3,A3)
   02 FORMAT('  ',I3,2X,A3,6I4,2I5)
   03 FORMAT(14I5)
   04 FORMAT (2H0 ,' NEQ = ',I5,'  NAUR = ',I5,'  IF = ',
     1I5,' IS = ',I5,' IT = ',I5,' ISEL = ',I5,' ICENT = ',I5,' NMUD = '0
     2 ,I5,' IDUMP = ',I5,' AIMPAS = ',I5,//)
   05 FORMAT(9F7.0,3F10.5,5A4,A3)
   06 FORMAT(20A4)
   07 FORMAT(1H0,11I5)
   09 FORMAT(9F8.5,I2,3X,A3)
   10 FORMAT(' ',I3,2X,A3,9F10.5,I5)
```

```
 11 FORMAT(1H ,6I5,6F10.5,2I5,A3)
 12 FORMAT(2H1 ,20A4)
 13 FORMAT(2H0 ,A3,' WAS NOT BOOTHED.(IPIC(3RD SUMMED) MAY BE TOO   ',
   1'LARGE.)...GUESS AGAIN...... ')
 15 FORMAT(2H0 ,'BOOTH VALUES:    NO   ATOM    IST SUMMED         2ND ',
   1'SUMMED          3RD SUMMED          MAX')
 27 FORMAT (2H0 ,9F3.0,3F10.5,5A4,A3)
351 FORMAT(///,30X,' FINAL FRACTIONAL COORDINATES PUNCHED AS FOLLOWS')
357 FORMAT(2H0,' THIS PROGRAM FINISHED NORMALLY')
375 FORMAT (2H0 ,'NO',2X,'ATOM',T14,'X',T24,'Y',T34,'Z',T44,'B11',
   1  T54,'B22',T64,'B33',T74,'B12',T84,'B13',T94,'B23',T102,'TABLE#',
   2//)
    READ(05,06)ITITLE
    WRITE(06,12) ITITLE
    READ(05,03)NEQ,NABR,IF,IS,IT,ISEL,ICENT,NMOD,IDUMP,ATMPAS
    WRITE(06,04) NEQ,NABR,IF,IS,IT,ISEL,ICENT,NMOD,IDUMP,ATMPAS
    READ(05,05)  ((PTW(M,N),M=1,12),(IDENT(M,N),M=1,6), N=1,NEQ)
    WRITE(06,27) ((PTW(M,N),M=1,12),(IDENT(M,N),M=1,6), N=1,NEQ)
    READ(05,02)  NV,NU,IORGN,NATOMS,IDISK
    WRITE(6,07)  NV,NU,IORGN,NATOMS,IDISK
    READ(05,01) (IPIC(I,1),IPIC(I,2),IPIC(I,3),NTRX(I),NTRY(I),NTRZ(I)
   1,B11(I),B22(I),B33(I),B12(I),B13(I),B23(I),LFT(I),NREO(I),CODW(I),
   2I=1,NATOMS)
    WRITE(06,11)(IPIC(I,1),IPIC(I,2),IPIC(I,3),NTRX(I),NTRY(I),NTRZ(I)
   1,B11(I),B22(I),B33(I),B12(I),B13(I),B23(I),LFT(I),NREO(I),CODW(I),
   2I=1,NATOMS)
    REWIND IDISK
     IVF=IORGN(IF)
    IVS=IORGN(IS)
     IVT=IORGN(IT)
C
     NF = NV(IF)
     NS = NV(IS)
     NT = NV(IT)
     NVF = NU(IF)
```

```
      NVS = NU(IS)
      NVT = NU(IT)
      READ(IDISK)  IRT,((PFS1(IRS,IRF),IRS=1,NVS),IRF=1,NVF)
      READ(IDISK)  IRT,((PFS2(IRS,IRF),IRS=1,NVS),IRF=1,NVF)
      READ(IDISK)  IRT,((PFS3(IRS,IRF),IRS=1,NVS),IRF=1,NVF)
      WRITE(06,15)
      NVTT = NVT - 2
       MVTT = NVTT + IVT
      IF(MVTT.GT.NT) MVTT = MVTT - NT
       DO 200 JLEVEL = 1,NVTT
      MLEVEL = IRT - 1
      IF (MLEVEL.GE.NT)  MLEVEL = MLEVEL - NT
      DO 198 NATS = 1,NATOMS
      IF(IPIC(NATS,IT).GT.MVTT) IPIC(NATS,IT) = MVTT
      IF (IPIC(NATS,IT).EQ.MLEVEL) GO TO 150
      GO TO 198
  150 CALL LOOK
      IF (IW(NATS).NE.MLEVEL) GO TO 198
      CALL BOOTH
  198 CONTINUE
      IF (JLEVEL.EQ.NVTT) GO TO 200
      DO 199 IRS = 1,NVS
      DO 199 IRF = 1,NVF
      PFS1(IRS,IRF) = PFS2(IRS,IRF)
      PFS2(IRS,IRF) = PFS3(IRS,IRF)
  199 CONTINUE
      READ(IDISK)  IRT,((PFS3(IRS,IRF),IRS=1,NVS),IRF=1,NVF)
  200 CONTINUE
      WRITE(06,07) IRT,MLEVEL,JLEVEL
      WRITE(06,375)
      WRITE(06,10)  (I,CODW(I),FC(I,1),FC(I,2),FC(I,3),B11(I),B22(I),
     1 B33(I),B12(I),B13(I),B23(I),LFT(I), I=1,NATOMS)
      DO 40 I = 1,NATOMS
      IF (TMAX(I).LE.0.0) WRITE(06,15) CODW(I)
      X(I) = FC(I,1) / NV(I)
```

```
      Y(I) = FC(I,2) / NV(2)
      Z(I) = FC(I,3) / NV(3)
   40 CONTINUE
      WRITE(06,375)
      WRITE(06,10) (I,CODW(I),X(I),Y(I),Z(I),B11(I),B22(I),B33(I),
     1B12(I),B13(I),B23(I),LFT(I),I = 1,NATOMS)
      DO 60 I = 1,NATOMS
      IF(NREQ(I).EQ.0) GO TO 554
      N = IABS(NREQ(I))
      ICI = 1
      IF (NREQ(I)) 545,550,550
  545 ICI = -1
  550 CONTINUE
      X(I) = ICI * (X(I) * PTW(1,N) + PTW(10,N))+ NTRX(I)
      Y(I) = ICI * ( Y(I) * PTW(5,N) + PTW(11,N))+ NTRY(I)
      Z(I) = ICI * ( Z(I) * PTW(9,N) + PTW(12,N))+ NTRZ(I)
      GO TO 60
  554 CONTINUE
       X(I) = X(I) + NTRX(I)
      Y(I) = Y(I) + NTRY(I)
      Z(I) = Z(I) + NTRZ(I)
   60 CONTINUE
  349 CONTINUE
      WRITE(06,351)
      WRITE(06,375)
      WRITE(06,10) (I,CODW(I),X(I),Y(I),Z(I),B11(I),B22(I),B33(I),
     1B12(I),B13(I),B23(I),LFT(I),I = 1,NATOMS)
       WRITE(07,09)  (X(I),Y(I),Z(I),B11(I),B22(I),B33(I),B12(I),B13(I),
     1 B23(I),LFT(I),CODW(I), I = 1,NATOMS)
      IF (AIMPAS.LE.0) GO TO 50
      REWIND 04
       WRITE(04,09)  (X(I),Y(I),Z(I),B11(I),B22(I),B33(I),B12(I),B13(I),
     1 B23(I),LFT(I),CODW(I), I = 1,NATOMS)
   50 CONTINUE
      WRITE(06,357)
```

```
  555 CONTINUE
      STOP
      END
C
C
                SUBROUTINE LOOK
C        THE PURPOSE OF THIS SUBROUTINE IS TO FIND THE  THE MAXIMUM F
C        IN THE CHOSEN 5X5X3 DIVISION VOLUME.
      DIMENSION IPIC(99,03),PFS1(60,120), PFS2(60,120), PFS3(60,120),
     1 TMAX(99), IU(99), IV(99), IW(99),FC(99,3)
      COMMON IPIC,NATS,IF,IS,II,IVF,IVS,IVT,TMAX,IU,IV,IW,PFS1,PFS2,
     1 PFS3, NF,NS,NT,FC,MLLVEL,NVS,NVF
      IPIC2 = IPIC(NATS,IS) - IVS + 1
      IPIC1 = IPIC(NATS,IF) - IVF + 1
      IF (IPIC2.LE.0) IPIC2 = IPIC2 + NS
      IF(IPIC1.LE.0) IPIC1 = IPIC1 + NF
      TMAX(NATS) =  PFS2(IPIC2,IPIC1)
      IV(NATS) = IPIC2 + IVS - 1
      IU(NATS) = IPIC1 + IVF - 1
      IW(NATS)= MLEVEL
      LG2 = NVS - 2
      IF (IPIC2.GT.LG2) IPIC2 = LG2
      LG1 = NVF  - 2
      IF (IPIC1.GT.LG1) IPIC1 = LG1
      IF (IPIC2.LT.3) IPIC2 = 3
      IF (IPIC1.LT.3) IPIC1 = 3
      DO 180 IMS = 1,3
      DO 180 ID2 = 1,5
      IPD2 = IPIC2 + ID2 - 3
      DO 180 ID1 = 1,5
      IPD1 = IPIC1 + ID1 - 3
      IF (IMS - 2) 152,154,156
  152 TRY = PFS3(IPD2,IPD1)
      IPD3 = MLLVLL + 1
      GO TO 160
```

```
  154 TRY = PFS2(IPD2,IPD1)
      IPD3 = MLEVEL
      GO TO 160
  156 TRY = PFS1(IPD2,IPD1)
      IPD3 = MLEVEL- 1
  160 IF(TMAX(NATS) - TRY) 175,180,180
  175 TMAX(NATS) = TRY
      IV(NATS)  = IPD2 + IVS - 1
      IU(NATS) = IPD1 + IVF - 1
      IW(NATS) = IPD3
  180 CONTINUE
      IF (IW(NATS).GT.MLEVEL) IPIC(NATS,IT) = IW(NATS)
      IF (IW(NATS).LT.MLEVEL) GO TO 190
      GO TO 191
  190 IV(NATS) = 0
      IW(NATS) = 0
      IU(NATS) = 0
      TMAX(NATS) = 0.0
      FC(NATS,1) = 0.0
      FC(NATS,2) = 0.0
      FC(NATS,3) = 0.0
  191 CONTINUE
      IF (IU(NATS).GE.NF) IU(NATS) = IU(NATS) - NF
      IF ( IV(NATS).GE.NS) IV(NATS) = IV(NATS) - NS
      IF (IW(NATS).GE.NT)   IW(NATS) = IW(NATS) - NT
      RETURN
      END
C
C
          SUBROUTINE BOOTH
C      THE PURPOSE OF THIS SUBROUTINE IS TO DETERMINE THE MAXIMUM F IN
C      THREE DIMENSIONS.
      DIMENSION IU(99), IV(99), IW(99), PFS1(60,120), PFS2(60,120),
     1 PFS3(60,120), FC(99,3),IPIC(99,3),TMAX(99),CCDW(99)
      COMMON IPIC,NATS,IF,IS,IT,IVF,IVS,IVT,TMAX,IU,IV,IW,PFS1,PFS2,
```

```
   1 PFS3, NF,NS,NT,FC,MLEVEL,NVS,NVF,CODW
     LIF = IU(NATS) - IVF + 1
     IF (LIF.LE.0) LIF = LIF + NF
     LIS = IV(NATS) - IVS + 1
     IF (LIF.LE.0) LIS = LIS + NS
     TMID = PFS2(LIS,LIF)
     TUPT = PFS3(LIS,LIF)
     TDNT = PFS1(LIS,LIF)
     TUPS = PFS2(LIS+1,LIF)
      TDNS = PFS2(LIS-1,LIF)
     TUPF = PFS2(LIS,LIF+1)
     TDNF = PFS2(LIS,LIF-1)
     IF (TUPF.GT.TDNF) GO TO 330
     TMAXF = TDNF
     TMINF = TUPF
     MINDF = LIF + IVF
     GO TO 335
 330 TMAXF = TUPF
     TMINF = TDNF
     MINDF = LIF + IVF - 2
 335 IF (MINDF.GT.NF) MINDF = MINDF - NF
     IF (TUPS.GT.TDNS) GO TO 340
     TMAXS = TDNS
     TMINS = TUPS
     MINDS = LIS + IVS
     GO TO 345
 340 TMAXS= TUPS
     TMINS = TDNS
     MINDS = LIS + IVS - 2
 345 IF (MINDS.GT.NS) MINDS = MINDS - NS
     IF (TUPT.GT.TDNT) GO TO 350
     TMAXT = TDNT
     TMINT = TUPT
     MINDT = IW(NATS) + 1
     GO TO 355
```

```
350 TMAXT = TUPT
    TMINT = TDNT
    MINDT = IW(NATS) - 1
355 IF (MINDT.GT.NT) MINDT = MINDT - NT
    RTBF = (TMAXF - TMINF) / (TMID - TMINF)
    RTBS = (TMAXS - TMINS) / (TMID - TMINS)
    RTBT = (TMAXT - TMINT) / (TMID - TMINT)
    BOOF = (RTBF - 4) / (2*RTBF - 4)
    BOOS = (RTBS - 4) / (2*RTBS - 4)
    BOOT = (RTBT - 4) / (2*RTBT - 4)
    IF (BOOF.LT.1.0.OR.BOOF.GT.1.5) TMAX(NATS) = 0.0
    IF (BOOS.LT.1.0.OR.BOOS.GT.1.5) TMAX(NATS) = 0.0
    IF (BOOT.LT.1.0.OR.BOOT.GT.1.5) TMAX(NATS) = 0.0
 14 FORMAT(1H ,14X,I5,3X,A3,I5,F10.5,'  /',I5,F10.5,'  /',I5,F10.5,
   12X,F10.1)
    WRITE(06,14)NATS,CUDA(NATS),IU(NATS),BOOF,IV(NATS),BOOS,IW(NATS),
   1BOOT,TMAX(NATS)
    FC1 = MINDF + BOOF
    FC2 = MINDS + BOOS
    FC3 = MINDT + BOOT
    IF (MINDF.GT.IU(NATS)) FC1 = MINDF - BOOF
    IF (MINDS.GT.IV(NATS)) FC2 = MINDS - BOOS
    IF (MINDT.GT.IW(NATS)) FC3 = MINDT - BOOT
    FC(NATS,IF) = FC1
    FC(NATS,IS) = FC2
    FC(NATS,IT) = FC3
    RETURN
    END
```

APPENDIX B

OBSERVED AND CALCULATED STRUCTURE FACTORS

Table B-1

Observed and Calculated Structure Factors for $C\ell Co(H_2dpg_2)$-(clan)$\cdot C_2H_5OH$

L	FO	FC
H= 0, K= 0		
2	2949	-3137
4	398	-473
6	-108	-115
8	401	485
10	-112	46
12	427	-435
14	530	556
16	-133	86
18	-131	-65
H= 0, K= 1		
1	485	649
2	1334	1295
3	440	-313
4	1079	1074
5	-111	100
6	1139	1080
7	-107	127
8	335	-347
9	189	-175
10	-112	-16
11	269	209
12	267	297
13	459	-459
14	694	-701
15	379	357
16	542	530
17	-135	50
18	-135	53
19	-142	30
H= 0, K= 2		
0	2055	-2207
1	1523	1485
2	461	334
3	195	-177
4	255	76
5	-111	48
6	-108	55
7	464	448
8	164	99
9	-108	24
10	401	379
11	-116	-20
12	287	202
13	301	-255
14	492	-512
15	-137	172
16	229	15
17	-133	-35
18	-135	-21
19	-143	19
H= 0, K= 3		
1	638	-561
2	982	-984
3	634	-828
4	218	-105
5	333	340
6	192	191
7	312	272
8	222	-229
9	-111	-27
10	189	189
11	-119	-106
12	185	72
13	196	123
14	210	150
15	376	-399
16	207	-130
17	-136	217
18	212	-67

L	FO	FC
19	-141	-100
H= 0, K= 4		
0	1749	1724
1	2748	-2742
2	211	-263
3	694	706
4	559	-557
5	181	-195
6	303	-279
7	210	-55
8	245	-234
9	-116	58
10	287	371
11	267	235
12	239	-203
13	267	289
14	-136	152
15	243	-247
16	-134	139
17	-135	-39
18	247	-216
H= 0, K= 5		
1	923	890
2	228	151
3	1038	-1034
4	-112	96
5	-111	14
6	228	209
7	593	-601
8	-117	87
9	337	326
10	448	-407
11	-126	-46
12	-132	-52
13	401	-441
14	240	19
15	658	676
16	-137	6
17	344	-306
18	-144	72
H= 0, K= 6		
0	629	622
1	1151	1149
2	424	-433
3	538	-535
4	-115	-147
5	437	445
6	275	226
7	377	369
8	-123	-37
9	439	-445
10	297	299
11	244	184
12	261	-173
13	350	-368
14	-136	-87
15	-138	130
16	-140	-134
17	230	225
H= 0, K= 7		
1	572	-596
2	-119	-130
3	318	328
4	554	-561
5	201	-187
6	488	539
7	-125	104
8	295	-323
9	-133	159
10	-135	70

L	FO	FC
11	-136	78
12	292	276
13	-137	-48
14	413	-407
15	288	-252
16	271	276
H= 0, K= 8		
0	-123	-23
1	-123	12
2	265	263
3	-129	79
4	-128	-152
5	439	-418
6	211	-107
7	-135	-66
8	241	217
9	-139	175
10	-142	-61
11	234	-134
12	-141	113
13	323	323
14	223	-137
15	-141	-109
H= 0, K= 9		
1	-130	168
2	-131	-130
3	-133	-55
4	-134	40
5	196	41
6	232	-132
7	-140	-59
8	247	198
9	-143	-172
10	-137	-81
11	-139	24
12	-140	47
13	235	57
14	-147	147
H= 0, K= 10		
0	428	433
1	274	225
2	216	-251
3	-140	-105
4	-141	133
5	229	169
6	-144	-152
7	-142	101
8	-143	-190
9	212	-148
10	283	299
11	-145	-54
12	222	-219
13	234	0
H= 0, K= 11		
1	-138	0
2	-140	176
3	-141	-141
4	269	-313
5	216	138
6	294	322
7	-141	-7
8	217	-160
9	-147	111
10	-151	-26
11	-151	9
H= 0, K= 12		
0	-139	-115
1	-143	170

L	FO	FC
2	-142	100
3	-146	-138
4	-144	-10
5	-145	-64
6	278	18
7	246	139
8	-150	67
H= 0, K= 13		
1	-146	-10
2	-146	-11
3	-146	121
4	-153	-55
H= 1, K= 0		
1	1980	-2098
3	844	833
5	419	442
7	1784	-1783
9	996	1025
11	-113	0
13	-124	179
15	282	350
17	211	-303
19	310	339
-19	-140	60
-17	192	-158
-15	619	614
-13	690	-696
-11	160	3
-9	398	-450
-7	-164	-177
-5	867	861
-3	1438	-1533
-1	2044	1892
H= 1, K= 1		
0	504	576
1	1395	1364
2	-98	50
3	1698	-1655
4	1269	1259
5	-114	16
6	557	-543
7	554	-547
8	-111	-40
9	-111	-151
10	-116	154
11	259	-277
12	200	-195
13	639	-656
14	471	512
15	716	685
16	-136	-185
17	231	-210
18	-138	68
19	-142	91
-19	-133	103
-18	-138	-67
-17	-135	-133
-16	295	257
-15	571	562
-14	281	-252
-13	217	-142
-12	-124	-173
-11	-118	43
-10	175	-216
-9	347	372
-8	403	-403
-7	1168	-1156
-6	843	861
-5	487	480
-4	1279	-1215
-3	354	-328
-2	-96	107

L	FO	FC
-1	585	-563

H= 1, K= 2

L	FO	FC
0	-101	-17
1	1167	1077
2	-107	-48
3	1256	1185
4	415	404
5	436	435
6	-110	10
7	-112	123
8	452	-474
9	-113	15
10	-115	46
11	-118	78
12	-123	78
13	489	-457
14	-135	-66
15	-137	-112
16	-134	12
17	-134	75
18	-135	3
19	-147	5
-19	246	-96
-18	-139	-120
-17	215	148
-16	-136	-203
-15	451	-404
-14	332	368
-13	491	490
-12	268	-255
-11	512	518
-10	-114	65
-9	546	-543
-8	627	-594
-7	374	388
-6	-109	-66
-5	204	96
-4	-114	-55
-3	2196	2056
-2	1663	-1663
-1	2235	-2404

H= 1, K= 3

L	FO	FC
0	2381	-2335
1	1050	1038
2	-118	-56
3	806	-833
4	1758	1710
5	-112	-144
6	228	-225
7	-111	-13
8	754	-729
9	707	702
10	-117	29
11	-123	-179
12	-136	234
13	-134	259
14	349	-359
15	252	-317
16	289	300
17	-139	-83
18	197	-209
19	-141	-32
-19	-145	-189
-18	228	47
-17	-138	98
-16	-136	-155
-15	229	-233
-14	244	215
-13	-130	-122
-12	182	84
-11	-117	85
-10	-116	-29
-9	386	-417
-8	-112	-163

L	FO	FC
-7	358	330
-6	-112	-72
-5	385	-327
-4	750	763
-3	474	502
-2	315	-280
-1	2463	-2419

H= 1, K= 4

L	FO	FC
0	981	-1005
1	-115	-169
2	844	828
3	501	-490
4	-112	51
5	206	-153
6	499	-490
7	584	-571
8	541	521
9	228	218
10	-123	-112
11	-129	-194
12	238	105
13	199	171
14	-138	-71
15	-139	147
16	-134	-113
17	310	-265
18	238	74
-19	-140	15
-18	-138	-84
-17	-134	-44
-16	-139	194
-15	-135	141
-14	580	-582
-13	-134	-94
-12	-134	199
-11	213	159
-10	440	415
-9	333	-324
-8	-113	-119
-7	221	146
-6	335	270
-5	610	614
-4	563	-534
-3	340	-370
-2	322	328
-1	621	591

H= 1, K= 5

L	FO	FC
0	574	538
1	212	-190
2	886	-886
3	-112	-85
4	671	672
5	-114	122
6	683	-705
7	343	341
8	222	81
9	389	-386
10	191	193
11	-132	25
12	323	-314
13	-139	35
14	569	587
15	257	-156
16	342	-374
17	230	171
18	-143	70
-18	323	-258
-17	-133	-6
-16	456	442
-15	-137	113
-14	362	-423
-13	-136	133
-12	-131	-123
-11	-130	-23

L	FO	FC
-10	-125	-36
-9	-119	-147
-8	404	-403
-7	-114	56
-6	1334	1319
-5	163	-54
-4	821	-858
-3	426	-412
-2	563	-594
-1	1052	1033

H= 1, K= 6

L	FO	FC
0	1459	1489
1	178	-4
2	301	-321
3	-117	150
4	-121	-239
5	-118	-5
6	514	501
7	268	-276
8	620	-616
9	351	353
10	438	428
11	223	-60
12	251	-289
13	-140	49
14	-135	48
15	-136	-81
16	-145	204
17	-145	3
-17	-143	-42
-16	-142	-73
-15	-136	180
-14	338	347
-13	255	-239
-12	411	-384
-11	388	450
-10	232	273
-9	258	-308
-8	-125	-46
-7	184	232
-6	387	-410
-5	-116	14
-4	999	1028
-3	492	-510
-2	1315	-1314
-1	277	282

H= 1, K= 7

L	FO	FC
0	290	292
1	534	552
2	-118	-150
3	212	-258
4	317	289
5	164	202
6	269	238
7	304	-268
8	-135	47
9	-136	102
10	343	-331
11	248	243
12	298	256
13	312	-302
14	256	-266
15	288	255
16	211	161
-17	221	-220
-16	-145	-169
-15	-142	132
-14	-134	0
-13	-137	-115
-12	273	246
-11	-137	63
-10	401	-410
-9	-133	87
-8	231	239

L	FO	FC
-7	369	-414
-6	-126	-108
-5	722	740
-4	515	516
-3	251	-270
-2	840	-839
-1	518	-570

H= 1, K= 8

L	FO	FC
0	-126	0
1	-126	61
2	-124	38
3	-126	57
4	-132	0
5	-138	-138
6	-136	-54
7	-138	-30
8	-142	61
9	-144	-216
10	-142	108
11	297	239
12	241	154
13	-139	-91
14	-146	-118
15	-146	12
-16	221	54
-15	-144	-147
-14	-141	-141
-13	270	297
-12	-138	17
-11	-138	-157
-10	-139	55
-9	-142	-38
-8	-141	-68
-7	-137	-60
-6	219	217
-5	-131	93
-4	218	-205
-3	259	320
-2	-129	75
-1	366	-440

H= 1, K= 9

L	FO	FC
0	-136	-111
1	-135	22
2	-134	-41
3	-134	46
4	-141	148
5	-145	-153
6	-145	-215
7	-146	109
8	-144	-59
9	207	-150
10	220	174
11	-145	-225
12	-143	-106
13	230	301
14	-146	96
-14	-142	19
-13	-139	-44
-12	267	-206
-11	249	201
-10	-140	95
-9	305	-257
-8	-142	-21
-7	377	393
-6	365	338
-5	-137	-116
-4	324	-334
-3	-138	-169
-2	-136	95
-1	195	204

H= 1, K= 10

L	FO	FC
0	251	176

L	FO	FC
1	-143	-186
2	-141	-59
3	-143	-3
4	-146	-1
5	242	231
6	-143	87
7	207	-145
8	294	-280
9	-143	174
10	-144	129
11	-146	-190
12	-145	42
-13	-145	-114
-12	-147	-22
-11	-145	173
-10	-140	-34
-9	-140	-147
-8	-140	-20
-7	-143	105
-6	-136	-3
-5	-147	224
-4	-148	166
-3	393	-369
-2	-145	-60
-1	398	411

H= 1, K= 11

L	FO	FC
0	-137	97
1	-140	125
2	-140	-98
3	370	-370
4	313	284
5	-149	292
6	-143	-142
7	-143	-89
8	-145	33
9	-148	-18
10	-149	-23
11	-153	183
-11	-151	-132
-10	-145	66
-9	-150	277
-8	288	-227
-7	306	-353
-6	-139	166
-5	209	240
-4	-135	-39
-3	-142	-139
-2	-138	-42
-1	-142	103

H= 1, K= 12

L	FO	FC
0	267	174
1	-143	97
2	-139	-38
3	-144	2
4	-148	-94
5	-145	-81
6	-146	159
7	-147	78
8	-151	-143
-8	-148	-191
-7	219	20
-6	-143	19
-5	-146	-126
-4	-143	55
-3	-146	87
-2	304	-206
-1	-143	-88

H= 1, K= 13

L	FO	FC
0	-150	-45
1	-153	66
2	-151	157
3	242	-16
4	-149	-138
-4	234	84
-3	-148	-29
-2	-151	-58
-1	-145	-79

H= 2, K= 0

L	FO	FC
0	592	569
2	922	-916
4	1131	1113
6	1893	-1823
8	1724	1697
10	758	-772
12	248	72
14	-137	125
16	562	-568
18	466	461
-20	-143	-131
-18	-136	-156
-16	557	565
-14	598	-626
-12	548	539
-10	444	-463
-8	372	-378
-6	454	444
-4	956	-957
-2	1126	1073

H= 2, K= 1

L	FO	FC
0	314	309
1	-100	-153
2	1529	-1525
3	209	-231
4	1255	1271
5	-112	-58
6	306	-258
7	387	380
8	359	-322
9	-114	2
10	382	373
11	417	-414
12	428	-435
13	336	346
14	504	555
15	-139	-161
16	-139	-340
17	-134	36
18	-136	-41
19	-145	89
-19	-138	-55
-18	350	-373
-17	220	170
-16	241	235
-15	245	-225
-14	-132	121
-13	-123	-52
-12	330	-292
-11	-113	29
-10	623	619
-9	581	-583
-8	1385	-1377
-7	602	591
-6	384	399
-5	1273	-1239
-4	180	78
-3	528	-491
-2	305	-272
-1	-98	29

H= 2, K= 2

L	FO	FC
0	-106	1
1	609	-620
2	1329	-1307
3	1240	-1223
4	209	-244
5	232	213
6	503	510
7	279	-312
8	-111	-94
9	-116	182
10	264	-301
11	222	-250
12	151	-71
13	259	-275
14	-130	-79
15	-135	141
16	257	237
17	200	-248
18	-144	-175
19	-145	64
-19	157	-81
-18	-141	158
-17	-135	-18
-16	425	-403
-15	258	254
-14	333	424
-13	254	-310
-12	314	284
-11	305	383
-10	-116	25
-9	-112	109
-8	200	-148
-7	204	100
-6	1075	-1056
-5	-112	-251
-4	-114	-73
-3	-113	-193
-2	508	672
-1	631	671

H= 2, K= 3

L	FO	FC
0	252	-257
1	400	409
2	320	298
3	161	-171
4	-112	61
5	522	563
6	-109	-24
7	-113	50
8	-114	-138
9	-117	110
10	238	-287
11	-126	21
12	279	236
13	262	-279
14	399	-413
15	245	323
16	-134	114
17	-142	-135
18	-138	-72
-19	-141	131
-18	-139	103
-17	272	-224
-16	-132	-182
-15	229	-163
-14	-135	-83
-13	213	164
-12	404	478
-11	-115	-165
-10	335	-328
-9	400	425
-8	461	402
-7	223	-209
-6	356	373
-5	-109	96
-4	272	-263
-3	803	790
-2	1252	-1228
-1	-117	-29

H= 2, K= 4

L	FO	FC
0	1324	-1259
1	403	-393
2	-113	-50
3	216	252
4	-112	250
5	234	-300
6	-113	-130
7	550	561
8	413	424
9	260	-281
10	-125	166
11	309	321
12	-133	-90
13	-139	88
14	-123	-4
15	-138	-171
16	-137	-54
17	-140	95
18	-140	127
-19	-140	-82
-18	-139	-15
-17	239	250
-16	-134	53
-15	379	-432
-14	215	-92
-13	358	373
-12	-127	127
-11	436	-431
-10	171	26
-9	-115	18
-8	-113	0
-7	269	224
-6	407	397
-5	250	-260
-4	-110	84
-3	-112	-184
-2	1520	1537
-1	-110	121

H= 2, K= 5

L	FO	FC
0	599	-620
1	881	-899
2	368	-344
3	575	550
4	-115	-95
5	393	-348
6	216	277
7	-116	11
8	319	-317
9	330	303
10	284	301
11	509	-567
12	-137	-116
13	726	726
14	-134	105
15	281	-251
16	-140	119
17	-139	43
18	-140	-96
-18	-138	-14
-17	-143	239
-16	157	146
-15	222	-217
-14	-134	-131
-13	221	-117
-12	315	-244
-11	439	470
-10	-127	144
-9	583	-560
-8	239	-195
-7	693	676
-6	-114	-66
-5	523	-539
-4	712	-703
-3	176	-185
-2	1140	1103
-1	1397	1369

L	FO	FC
H= 2, K= 6		
0	269	-293
1	646	-625
2	584	-576
3	-119	-168
4	203	79
5	748	786
6	197	-204
7	541	-542
8	258	275
9	337	334
10	319	-365
11	-133	13
12	-145	-5
13	-141	-120
14	-135	56
15	-137	81
16	-139	-58
17	-145	-117
-17	-145	-194
-16	-137	208
-15	347	344
-14	-141	-253
-13	310	-308
-12	421	416
-11	204	210
-10	360	-358
-9	-128	58
-8	199	256
-7	262	-294
-6	-122	-92
-5	-120	246
-4	532	-517
-3	609	-601
-2	1065	1096
-1	1220	1224
H= 2, K= 7		
0	601	579
1	206	210
2	394	-435
3	375	-341
4	449	465
5	-130	151
6	-132	-277
7	-136	-152
8	-133	60
9	-138	-139
10	222	226
11	335	347
12	572	-601
13	255	-188
14	306	308
15	-147	152
16	215	-71
-17	-146	-97
-16	-143	89
-15	200	16
-14	-136	85
-13	219	126
-12	-138	-170
-11	219	-257
-10	457	455
-9	403	441
-8	476	-503
-7	240	-315
-6	437	459
-5	189	-150
-4	-124	72
-3	-122	153
-2	382	-410
-1	299	-221
H= 2, K= 8		
0	195	-153
1	-133	300
2	-130	-4
3	285	290
4	-134	-124
5	-135	-142
6	-141	198
7	-142	-89
8	-141	56
9	217	-162
10	213	127
11	-141	7
12	-139	-131
13	-144	-6
14	-141	-9
15	-144	121
-16	281	-187
-15	-148	-45
-14	-143	128
-13	-137	60
-12	-136	-88
-11	-141	152
-10	-145	181
-9	-147	-284
-8	-140	-161
-7	380	415
-6	-134	-34
-5	-134	-85
-4	481	499
-3	280	304
-2	-129	-129
-1	425	-431
H= 2, K= 9		
0	291	-369
1	-137	-52
2	-141	145
3	-137	79
4	-137	0
5	231	241
6	-143	-42
7	-146	-126
8	-144	-38
9	-142	183
10	-138	-31
11	-143	-271
12	236	223
13	-151	138
14	-149	-72
-14	-139	-8
-13	-143	-66
-12	-141	34
-11	313	257
-10	224	-310
-9	252	-228
-8	-140	25
-7	-140	117
-6	-140	71
-5	285	-275
-4	-138	-68
-3	509	507
-2	263	377
-1	301	-252
H= 2, K= 10		
0	276	-243
1	-142	-146
2	-146	-77
3	-143	-99
4	-147	188
5	-145	153
6	300	-262
7	-141	-3
8	-145	196
9	-143	81
10	-149	-216
11	-146	-15
12	-146	55
-13	-147	-88
-12	-144	111
-11	-144	-55
-10	-142	5
-9	-140	206
-8	-140	-98
-7	-141	-74
-6	-139	-25
-5	-148	-148
-4	370	-355
-3	-143	19
-2	488	487
-1	201	226
H= 2, K= 11		
0	-144	198
1	-143	-73
2	330	-352
3	-143	62
4	307	324
5	-143	-186
6	-144	-73
7	-145	177
8	-146	-112
9	-149	-29
10	327	240
-11	322	163
-10	-152	230
-9	-144	-146
-8	292	-355
-7	-144	119
-6	331	270
-5	-142	-102
-4	-143	13
-3	-140	-26
-2	-144	-220
-1	-142	105
H= 2, K= 12		
0	-144	126
1	-145	-6
2	-147	-35
3	214	-107
4	-149	-163
5	-149	224
6	254	144
7	226	-249
8	223	-42
-8	-151	-17
-7	-149	-29
-6	-153	-122
-5	-151	251
-4	225	277
-3	335	-359
-2	-145	-177
-1	282	223
H= 2, K= 13		
0	-149	53
1	-150	104
2	-148	15
3	-148	-71
-4	-150	-59
-3	-151	52
-2	-151	-8
-1	278	-188
H= 3, K= 0		
1	586	-564
3	799	-796
5	1501	-1510
7	1092	1081
9	494	-493
11	273	-247
13	408	429
15	714	-729
17	294	304
19	254	-155
-19	-136	-64
-17	613	634
-15	531	-542
-13	497	493
-11	440	-436
-9	356	-310
-7	1011	1026
-5	1442	-1403
-3	203	221
-1	1290	-1240
H= 3, K= 1		
0	551	-573
1	289	-216
2	1796	1738
3	281	-271
4	583	-589
5	241	-271
6	754	-771
7	510	-492
8	-114	124
9	716	708
10	-121	-169
11	796	-805
12	343	389
13	446	432
14	307	-268
15	199	-127
16	215	-187
17	-136	-102
18	-141	27
19	-146	150
-19	-144	-179
-18	213	130
-17	-137	232
-16	-135	-103
-15	-138	196
-14	-129	-88
-13	412	-424
-12	-125	194
-11	885	870
-10	270	-286
-9	453	-438
-8	624	615
-7	282	241
-6	333	-399
-5	-110	179
-4	505	-520
-3	-112	48
-2	393	323
-1	1687	1683
H= 3, K= 2		
0	450	-470
1	413	385
2	822	849
3	222	-194
4	852	831
5	1072	1074
6	635	-636
7	428	-421
8	428	446
9	190	238
10	-117	-94
11	-122	-173
12	184	-116
13	-134	-217
14	337	339
15	-141	251
16	280	-219

L	FO	FC
17	-136	-185
18	285	127
-19	-140	95
-18	242	-216
-17	225	-273
-16	-136	160
-15	421	420
-14	302	-229
-13	-129	-197
-12	416	449
-11	402	-409
-10	-114	49
-9	516	522
-8	554	-529
-7	172	-156
-6	553	547
-5	202	-220
-4	-112	-16
-3	210	-161
-2	654	610
-1	369	-330

H= 3, K= 3

L	FO	FC
0	-115	-9
1	331	-281
2	1146	1182
3	298	-331
4	485	-444
5	428	428
6	-112	95
7	162	72
8	217	244
9	-117	-29
10	328	260
11	257	256
12	335	-309
13	221	-222
14	-138	193
15	-137	199
16	-132	159
17	-139	-83
18	-143	-74
-19	-140	89
-18	-138	13
-17	-135	-80
-16	-135	-193
-15	-133	-97
-14	-132	99
-13	315	324
-12	338	-328
-11	496	-505
-10	636	649
-9	352	367
-8	-112	-34
-7	-109	-78
-6	516	-555
-5	-110	-103
-4	275	-270
-3	557	566
-2	411	-380
-1	849	-841

H= 3, K= 4

L	FO	FC
0	199	-205
1	549	535
2	-109	-23
3	-112	-7
4	504	-510
5	529	-560
6	359	389
7	-117	85
8	208	-160
9	246	319
10	209	93
11	288	-231
12	-137	140

L	FO	FC
13	248	179
14	281	-300
15	-136	-189
16	-145	166
17	-147	192
18	-145	-165
-19	-143	75
-18	278	244
-17	-138	-25
-16	421	-406
-15	-135	-34
-14	255	267
-13	-130	94
-12	220	24
-11	-125	-8
-10	-121	-121
-9	-119	-224
-8	598	608
-7	245	283
-6	248	233
-5	232	-186
-4	-110	-36
-3	579	603
-2	738	-778
-1	858	-858

H= 3, K= 5

L	FO	FC
0	587	-574
1	219	47
2	940	967
3	-113	-47
4	710	-718
5	-118	-152
6	280	-277
7	181	-158
8	386	398
9	187	228
10	380	-379
11	-134	34
12	636	638
13	-137	64
14	218	-210
15	-140	-214
16	-137	-97
17	-140	-8
-18	273	247
-17	254	220
-16	-136	-48
-15	223	-246
-14	-136	-162
-13	-140	181
-12	-135	162
-11	-132	-27
-10	628	-629
-9	-119	39
-8	969	954
-7	-115	7
-6	200	53
-5	-115	-7
-4	358	-339
-3	-113	91
-2	1008	1015
-1	293	-268

H= 3, K= 6

L	FO	FC
0	-118	96
1	302	280
2	531	-538
3	268	264
4	659	651
5	678	-694
6	847	-851
7	372	398
8	413	451
9	290	-288
10	-135	-166

L	FC	FC
11	-140	51
12	258	-220
13	373	378
14	374	318
15	-144	-177
16	-150	-210
-17	-147	129
-16	324	307
-15	-137	49
-14	378	-337
-13	-138	19
-12	271	314
-11	-136	-196
-10	236	192
-9	-124	-7
-8	525	-500
-7	538	523
-6	-120	191
-5	407	-407
-4	573	-582
-3	316	314
-2	893	920
-1	-114	44

H= 3, K= 7

L	FO	FC
0	633	626
1	466	-456
2	288	253
3	443	472
4	-123	-11
5	-128	-38
6	-130	29
7	183	-102
8	-135	-83
9	-141	22
10	203	156
11	242	-235
12	353	-377
13	-143	194
14	-140	195
15	-143	-16
16	-144	-2
-16	-143	-33
-15	-139	-9
-14	-136	39
-13	-135	-57
-12	243	-204
-11	318	248
-10	314	287
-9	561	-558
-8	-134	163
-7	-133	110
-6	274	-148
-5	-126	86
-4	294	350
-3	447	-470
-2	646	-672
-1	524	546

H= 3, K= 8

L	FO	FC
0	330	412
1	194	46
2	-134	4
3	-133	-170
4	257	-181
5	247	208
6	-137	164
7	-140	-178
8	-145	242
9	-142	69
10	-142	-79
11	-137	1
12	209	-52
13	-141	-196
14	-144	18
15	230	97

L	FO	FC
-15	-146	82
-14	-128	2
-13	-137	101
-12	236	142
-11	-141	-125
-10	385	-390
-9	-139	116
-8	-140	207
-7	-136	-110
-6	-135	-22
-5	-138	258
-4	260	280
-3	590	-574
-2	447	-490
-1	-129	84

H= 3, K= 9

L	FO	FC
0	-137	-79
1	228	102
2	-141	131
3	-139	-82
4	-137	-36
5	-144	93
6	286	-323
7	241	75
8	221	213
9	232	-157
10	-144	-67
11	-145	67
12	217	273
13	-151	-70
-14	222	147
-13	-144	6
-12	-140	-41
-11	-140	-66
-10	-141	-128
-9	-141	138
-8	-144	-9
-7	-142	101
-6	263	198
-5	-139	-170
-4	294	-245
-3	285	329
-2	-138	43
-1	352	-366

H= 3, K= 10

L	FO	FC
0	266	-172
1	-147	-10
2	-147	60
3	-146	91
4	-147	-29
5	315	-292
6	-148	10
7	239	253
8	-147	-136
9	-149	-48
10	-148	35
11	-152	50
12	-152	52
-13	-152	87
-12	-154	244
-11	-151	-146
-10	-146	-78
-9	-145	-37
-8	278	-159
-7	-152	284
-6	-144	64
-5	357	-379
-4	-151	-88
-3	349	386
-2	262	327
-1	-145	-134

L	FO	FC
H=	3, K=	11
0	-147	-69
1	-156	-318
2	-146	86
3	-151	151
4	-147	-126
5	266	25
6	-150	146
7	-153	-226
8	-149	-32
9	-161	248
10	-155	-109
-11	-153	3
-10	-150	-43
-9	-149	-41
-8	-149	186
-7	-148	-51
-6	-150	-52
-5	-146	-47
-4	379	-395
-3	296	-279
-2	299	333
-1	521	524
H=	3, K=	12
0	-151	-123
1	-147	-33
2	-153	-44
3	-149	3
4	-155	115
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9	-123	4
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-17	-144	-200
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16	-142	112
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-16	-138	-199
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8	219	-346
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11	241	-272
12	-139	179
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14	-128	-168
15	298	-224
16	-143	108
-17	295	277
-16	-140	14
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-14	-134	-218
-13	-136	20
-12	-136	56
-11	251	197
-10	377	-377
-9	349	-354
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6	345	-310
7	397	-388
8	399	413
9	-143	192
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11	313	-238
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13	330	324
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15	-147	-114
-16	-146	75
-15	-136	-14
-14	-140	-44
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-12	-140	-20
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-10	-142	-207
-9	226	-232
-8	206	212
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12	-140	-164
13	-143	-185
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-15	-145	111
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-13	-140	50
-12	-137	-185
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3	257	141
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-9	-146	-13
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-17	299	284
-15	-137	-261
-13	-132	-160
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-7	1354	-1369
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7	662	644
8	375	-380
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10	372	365
11	292	366
12	-132	64
13	404	-409
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15	-137	113
16	-136	96
17	407	401
18	-148	-155
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-18	-138	-160
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-16	208	139
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-12	-127	-61
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-9	-113	17
-8	369	-344
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15	-138	49
16	-135	146
17	-122	20
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-19	269	-293
-18	-144	220
-17	245	37
-16	-133	-43
-15	-137	-115
-14	269	-291
-13	262	-200
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-11	762	735
-10	315	-295
-9	211	-157
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7	326	-363
8	520	508
9	368	434
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11	-130	63
12	156	-174
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15	158	-65
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-18	-139	-35
-17	-137	-143
-16	-133	15
-15	226	-196
-14	-135	-10
-13	224	-126
-12	334	334
-11	-122	32
-10	184	237
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5	472	-451
6	-118	-134
7	474	-466
8	450	-470
9	-128	-39
10	383	375
11	-137	104
12	-138	186
13	235	-153
14	-137	-98
15	-141	58
16	-140	-16
17	-143	41
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-17	235	-17
-16	-139	-105
-15	232	353
-14	237	188
-13	587	-610
-12	342	-382
-11	215	119
-10	438	430
-9	322	300
-8	208	-179
-7	222	-371
-6	605	611
-5	390	-410
-4	-114	56
-3	403	384
-2	-111	-33
-1	-114	168
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4	890	-895
5	209	-132
6	1020	1068
7	-125	48
8	1006	-1040
9	-132	0
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11	-137	72
12	384	-297
13	-136	-145
14	205	212
15	-138	60
16	-145	35
-18	-148	163
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-16	-139	-165
-15	-133	-10
-14	-141	159
-13	219	218
-12	573	-598
-11	-133	-97
-10	570	563
-9	-128	2
-8	-125	-155
-7	197	-137
-6	866	-888
-5	550	561
-4	747	784
-3	167	-129
-2	-115	-60
-1	213	-273

L	FU	FC
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2	521	548
3	378	-398
4	505	-484
5	378	392
6	240	173
7	-130	152
8	-134	151
9	-140	-248
10	462	-462
11	257	247
12	291	287
13	-138	-76
14	299	-291
15	-146	72
16	-149	160
-17	308	-179
-16	-139	-166
-15	-138	-168
-14	228	190
-13	263	202
-12	224	239
-11	280	-282
-10	559	-564
-9	190	149
-8	472	492
-7	273	-339
-6	438	-421
-5	-121	131
-4	209	136
-3	437	-453
-2	-120	102
-1	-119	114
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2	195	-88
3	-132	-24
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5	281	-291
6	381	-393
7	440	499
8	514	507
9	408	-384
10	237	-80
11	-135	62
12	-136	-165
13	-137	148
14	-143	-125
15	-146	-141
-16	-149	76
-15	-145	-152
-14	-136	-41
-13	-131	58
-12	-132	109
-11	-135	-85
-10	-137	-47
-9	-135	82
-8	212	-186
-7	-133	-90
-6	338	292
-5	259	-272
-4	297	-297
-3	256	294
-2	-127	130
-1	335	-305
H= 5, K= 8		
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1	235	-232
2	-136	-152
3	-142	265

L	FC	FC
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5	292	-327
6	-140	126
7	-143	87
8	-140	0
9	-145	83
10	-138	66
11	238	-254
12	-138	17
13	-151	107
14	-142	75
-15	-141	12
-14	-141	-33
-13	-141	-190
-12	-136	-73
-11	279	304
-10	-142	95
-9	-141	-171
-8	-142	-160
-7	-140	67
-6	216	-214
-5	-137	-180
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-3	-138	4
-2	490	-531
-1	276	261
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2	-146	-128
3	225	-113
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5	-150	221
6	-145	89
7	-141	-176
8	260	-197
9	-142	88
10	-144	66
11	212	-124
12	-144	65
-14	-148	123
-13	232	-82
-12	-146	-84
-11	-141	132
-10	-141	69
-9	-141	-20
-8	-144	-36
-7	-143	-55
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-5	-144	243
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-3	236	-249
-2	-138	24
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2	-143	101
3	325	-328
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6	-144	159
7	-142	-43
8	-142	-66
9	-147	-103
10	-150	-85
11	-154	289
-12	209	-52
-11	354	-320
-10	-143	-8
-9	521	505
-8	-137	41
-7	-143	-195
-6	-140	-151

L	FO	FC
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-4	-143	98
-3	-139	-8
-2	-145	24
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H= 5, K= 11		
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4	-144	-165
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7	314	263
8	-149	-21
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-9	-150	98
-8	-142	-1
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-5	-143	-3
-4	-137	-34
-3	-143	103
-2	-142	-10
-1	-146	-237
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3	-147	107
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5	-154	-19
-7	-153	100
-6	-152	-140
-5	-144	62
-4	-146	54
-3	-153	-157
-2	-151	93
-1	-149	79
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4	1232	1246
6	299	-254
8	603	-619
10	1064	1071
12	-132	-21
14	-135	66
16	-139	-46
-18	334	-321
-16	-130	42
-14	-136	-102
-12	715	-744
-10	832	850
-8	-112	-158
-6	1003	988
-4	-109	119
-2	-108	-49
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3	156	-137
4	2108	-2038
5	323	269
6	605	615
7	181	-111
8	248	-337
9	264	336
10	261	252

L	FO	FC
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12	-135	-137
13	217	-22
14	-130	64
15	215	186
16	395	372
17	-145	-126
-19	-144	21
-18	331	285
-17	-137	56
-16	-134	101
-15	-135	-54
-14	343	-351
-13	-130	60
-12	-129	-43
-11	-125	-77
-10	258	-257
-9	232	-174
-8	242	241
-7	389	416
-6	1776	-1745
-5	851	839
-4	1957	1926
-3	962	-958
-2	-109	-24
-1	-110	57

H= 6, K= 2

L	FO	FC
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2	993	991
3	995	-988
4	221	-198
5	273	-280
6	471	-445
7	254	-226
8	234	-68
9	-123	-69
10	-129	-3
11	-131	18
12	313	-250
13	-138	26
14	-140	247
15	-133	-116
16	-138	7
17	236	196
-19	-146	189
-18	-138	-40
-17	216	-228
-16	-136	95
-15	327	320
-14	253	194
-13	-130	-41
-12	211	239
-11	402	-419
-10	412	-417
-9	-120	123
-8	-114	183
-7	-111	2
-6	534	517
-5	154	36
-4	1414	-1398
-3	213	219
-2	-108	-70
-1	200	236

H= 6, K= 3

L	FO	FC
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5	844	-853
6	-120	89
7	-117	74
8	-124	-71
9	206	-83
10	-133	-232
11	-134	21
12	310	-206
13	315	-216
14	-136	168
15	-140	77
16	-143	-192
17	-149	178
-18	250	-251
-17	-138	69
-16	-139	31
-15	253	217
-14	202	-170
-13	-134	45
-12	-131	-16
-11	-129	-45
-10	351	401
-9	400	-405
-8	-120	185
-7	621	655
-6	-111	56
-5	569	-544
-4	399	-397
-3	268	248
-2	167	-13
-1	214	254

H= 6, K= 4

L	FO	FC
0	230	267
1	184	-163
2	508	-502
3	550	533
4	523	488
5	-120	-92
6	-125	29
7	-127	50
8	-127	8
9	305	313
10	-136	143
11	288	-349
12	-136	125
13	-142	105
14	-136	-64
15	-144	37
16	-140	-104
-18	-142	-23
-17	-139	-15
-16	234	84
-15	-134	126
-14	383	-365
-13	423	-431
-12	-139	-126
-11	481	458
-10	-129	45
-9	389	-370
-8	-120	-101
-7	-120	60
-6	621	607
-5	191	41
-4	295	-244
-3	433	-431
-2	242	-252
-1	-115	35

H= 6, K= 5

L	FO	FC
0	218	139
1	175	181
2	-118	-46
3	572	-599
4	-125	-203
5	637	659
6	-127	-81
7	553	-574
8	-136	-214
9	319	318
10	256	222
11	-141	68
12	-144	165
13	253	-142
14	-131	-61
15	-142	39
16	-141	115
-17	-141	-30
-16	-136	13
-15	201	146
-14	-137	50
-13	213	-276
-12	234	-237
-11	-121	-41
-10	-122	-10
-9	-132	181
-8	-128	-131
-7	406	-402
-6	174	-170
-5	954	1008
-4	178	103
-3	1125	-1141
-2	-119	-131
-1	-117	72

H= 6, K= 6

L	FO	FC
0	346	372
1	418	450
2	185	-232
3	590	-607
4	306	256
5	-133	43
6	-133	-152
7	280	225
8	385	-357
9	263	-320
10	228	231
11	366	430
12	358	-345
13	-141	-77
14	-145	36
15	-146	61
-17	-143	-6
-16	-146	201
-15	-140	20
-14	-135	52
-13	-136	95
-12	236	-225
-11	367	-372
-10	258	233
-9	270	312
-8	-122	-75
-7	357	-349
-6	-130	0
-5	187	19
-4	-123	-136
-3	542	546
-2	447	-470
-1	237	-305

H= 6, K= 7

L	FO	FC
0	219	221
1	-135	-76
2	-135	131
3	257	274
4	314	-332
5	333	-350
6	221	319
7	204	226
8	-141	-97
9	268	-278
10	221	204
11	-142	-151
12	-140	-65
13	-146	263
14	-152	-170
-16	-148	-46
-15	-145	-115
-14	-140	127
-13	297	253
-12	-140	-174
-11	-137	102
-10	284	302
-9	419	-454
-8	-139	181
-7	-137	100
-6	-143	-238
-5	-137	-214
-4	354	403
-3	-136	-87
-2	214	-256
-1	-131	151

H= 6, K= .8

L	FO	FC
0	-140	-108
1	-140	-61
2	-142	253
3	-140	-63
4	-141	-69
5	258	155
6	-141	-57
7	-143	156
8	-141	147
9	-142	-128
10	-145	-196
11	198	-91
12	257	235
13	-149	-151
-15	-148	40
-14	-145	-206
-13	-143	-96
-12	218	236
-11	-147	249
-10	370	-356
-9	-145	163
-8	-138	65
-7	248	55
-6	247	272
-5	-140	-114
-4	-139	-153
-3	338	-362
-2	206	124
-1	296	276

H= 6, K= 9

L	FO	FC
0	211	102
1	-144	31
2	259	-187
3	-145	-135
4	320	248
5	255	206
6	-140	-146
7	250	-134
8	-143	86
9	213	191
10	-147	-8
11	-149	66
-13	239	-182
-12	-144	73
-11	-140	-97
-10	-139	196
-9	-146	232
-8	358	-328
-7	-141	-12
-6	-141	37
-5	-146	214
-4	-140	-69
-3	-143	-80
-2	-146	44
-1	-143	-47

H= 6, K= 10

L	FO	FC
0	-144	258
1	-143	77
2	208	-179
3	-143	-43
4	-141	113
5	-138	54
6	-144	-30
7	-147	-189
8	-146	-131
9	-147	92
10	254	266
-11	-150	22
-10	384	311
-9	-142	-152
-8	-142	-107
-7	-140	-51
-6	-136	105
-5	-147	174
-4	-143	-13
-3	-141	-38
-2	-144	-254
-1	-140	-81

H= 6, K= 11

L	FO	FC
0	-139	60
1	-143	33
2	-147	-32
3	-143	-24
4	278	-179
5	-147	59
6	-155	215
7	-150	-76
-9	-149	3
-8	-151	110
-7	-148	-56
-6	250	-219
-5	-148	73
-4	266	245
-3	-145	-61
-2	-142	-62
-1	-146	9

H= 6, K= 12

L	FO	FC
0	226	-74
1	238	189
2	267	179
3	226	-168
4	-150	-87
-5	-153	-1
-4	252	-23
-3	-144	29
-2	-150	95
-1	-148	-118

H= 7, K= 0

L	FO	FC
1	1005	-1026
3	-110	25
5	240	270
7	568	-555
9	889	906
11	557	-576
13	266	238
15	-137	-144
17	-150	-234
-17	-143	84
-15	-137	-117
-13	220	-208
-11	651	653
-9	380	-346
-7	-117	-155
-5	1071	1044
-3	799	-810
-1	-110	174

H= 7, K= 1

L	FO	FC
0	524	-538
1	673	654
2	581	-597
3	971	-971
4	613	589
5	-118	151
6	294	-363
7	263	-277
8	-126	132
9	-132	-55
10	252	-269
11	484	507
12	-139	106
13	318	-308
14	-138	70
15	-137	83
16	-139	-106
-18	248	-127
-17	-139	-52
-16	200	186
-15	-134	-158
-14	371	-376
-13	270	238
-12	345	409
-11	304	-312
-10	179	-12
-9	463	449
-8	411	-361
-7	830	-829
-6	-117	185
-5	1138	1106
-4	-112	58
-3	-110	-41
-2	724	741
-1	-112	-16

H= 7, K= 2

L	FO	FC
0	447	466
1	185	236
2	288	-264
3	249	-272
4	190	209
5	-117	-66
6	-118	165
7	464	471
8	300	-342
9	422	-415
10	335	305
11	-134	-23
12	-140	-208
13	-137	237
14	-140	-16
15	-139	90
16	-140	68
-18	-145	8
-17	-141	75
-16	-135	-7
-15	370	-353
-14	217	-244
-13	421	410
-12	210	-199
-11	271	-345
-10	376	390
-9	-118	48
-8	330	-361
-7	269	-254
-6	228	-209
-5	-112	-156
-4	298	338
-3	558	585
-2	-113	-95
-1	-110	164

H= 7, K= 3

L	FO	FC
0	385	-442
1	269	-305
2	370	323
3	-115	160
4	-116	-21
5	253	-287
6	-119	26
7	-124	106
8	229	193
9	-133	-64
10	-134	-20
11	294	-285
12	-139	24
13	-136	-7
14	-138	125
15	-137	-63
16	-142	111
-18	212	119
-17	-138	72
-16	-138	-2
-15	258	148
-14	-137	-79
-13	204	-216
-12	-137	219
-11	-128	50
-10	508	-522
-9	421	-421
-8	-122	182
-7	444	446
-6	407	-408
-5	490	-513
-4	275	298
-3	537	-528
-2	-111	-12
-1	449	475

H= 7, K= 4

L	FO	FC
0	215	-236
1	750	-763
2	-116	-97
3	652	638
4	271	289
5	329	-275
6	351	-324
7	-127	48
8	230	128
9	-132	-19
10	562	-576
11	-138	176
12	229	227
13	-139	-238
14	-136	-6
15	-145	-9
16	-150	-25
-17	-144	-30
-16	-139	25
-15	-134	14
-14	-141	-175
-13	-138	11
-12	418	407
-11	314	338
-10	437	-480
-9	366	-358
-8	-122	-32
-7	331	375
-6	547	525
-5	341	-312
-4	581	-616
-3	-116	191
-2	205	-104
-1	248	218

H= 7, K= 5

L	FO	FC
0	-121	-60
1	349	-325
2	697	-735
3	-126	157
4	840	862
5	-130	177
6	311	-318
7	-134	-228
8	-136	119
9	-137	-170
10	199	188
11	406	412
12	391	-410
13	195	-97
14	-145	216
15	-143	-53
-17	-146	97
-16	-141	47
-15	-141	-189
-14	-134	1
-13	235	150
-12	234	9
-11	220	78
-10	271	330
-9	284	-251
-8	656	-657
-7	-126	-1
-6	725	722
-5	264	302
-4	300	-338
-3	-122	145
-2	241	257
-1	-118	72

H= 7, K= 6

L	FO	FC
0	538	559
1	206	-199
2	361	-357
3	-132	147
4	-132	129
5	249	135
6	-134	-25
7	-140	-164
8	332	-341
9	223	209
10	578	559
11	268	-290
12	-139	-98
13	257	221
14	-143	-168
-16	-141	-146
-15	-141	-91
-14	310	248
-13	-137	87
-12	382	-389
-11	321	329
-10	405	402
-9	-137	-280
-8	310	-332
-7	252	-243
-6	296	259
-5	191	155
-4	201	204
-3	-127	-82
-2	497	-522
-1	271	353

H= 7, K= 7

L	FO	FC
0	416	-461
1	-133	165
2	-139	244
3	393	-397
4	-138	-92
5	336	362
6	-144	119
7	-141	-63
8	-136	9

L	FO	FC
9	-141	91
10	220	-212
11	-134	-111
12	-144	103
13	-146	-17
-15	-146	128
-14	-144	-58
-13	214	-156
-12	265	268
-11	-136	64
-10	474	-431
-9	222	238
-8	246	308
-7	257	-202
-6	259	-225
-5	-136	56
-4	-134	170
-3	251	-293
-2	-140	269
-1	282	235

H= 7, K= 8

L	FO	FC
0	-142	18
1	-139	-63
2	-140	50
3	211	65
4	-142	24
5	-144	-185
6	-141	24
7	-143	243
8	-136	128
9	266	-232
10	-141	-16
11	-143	147
12	224	-134
-14	-146	-166
-13	-150	248
-12	-139	95
-11	-144	-170
-10	198	-129
-9	-139	44
-8	-140	32
-7	-140	74
-6	-145	176
-5	-144	-218
-4	-138	-117
-3	276	235
-2	-139	59
-1	-141	-155

H= 7, K= 9

L	FO	FC
0	-141	-69
1	-144	-152
2	-139	-113
3	-142	177
4	230	183
5	-137	-99
6	-141	-135
7	-137	6
8	-141	66
9	-144	12
10	-144	50
11	-146	-5
-13	-143	0
-12	-143	13
-11	250	134
-10	-144	0
-9	228	-233
-8	-141	-139
-7	439	471
-6	-143	23
-5	-143	[illegible]
-4	-144	-13
-3	-144	[illegible]
-2	222	68
-1	-143	123

H= 7, K= 10

L	FO	FC
0	-139	74
1	-138	-149
2	-140	-128
3	-141	155
4	-145	138
5	-143	36
6	-140	-113
7	-150	-272
8	-148	40
9	226	258
-11	-149	201
-10	-148	73
-9	-144	-149
-8	-144	-125
-7	-139	-49
-6	-143	109
-5	206	169
-4	-142	19
-3	-140	-110
-2	-143	-125
-1	-142	191

H= 7, K= 11

L	FO	FC
0	-145	-20
1	208	145
2	-149	-8
3	-152	-146
4	-147	16
5	244	195
6	-149	-70
-8	-148	-82
-7	-149	-180
-6	-148	148
-5	226	198
-4	-147	-91
-3	-146	-241
-2	-142	77
-1	-140	-27

H= 7, K= 12

L	FO	FC
0	231	226
1	226	-73
-3	231	134
-2	284	-214
-1	-149	-82

H= 8, K= 0

L	FO	FC
0	275	-245
2	-115	119
4	180	130
6	740	-725
8	766	774
10	552	-564
12	193	176
14	-135	76
16	419	-370
-18	198	-133
-16	-137	25
-14	810	-805
-12	759	776
-10	-127	-173
-8	-122	82
-6	-115	89
-4	691	-680
-2	979	996

H= 8, K= 1

L	FO	FC
0	365	405
1	246	-327
[illegible]	403	-419
[illegible]	[illegible]34	319

L	FO	FC
4	435	394
5	440	-424
6	-132	-58
7	-126	156
8	224	-286
9	-133	80
10	644	663
11	-139	-65
12	356	-407
13	-132	23
14	294	290
15	-142	-87
16	270	-185
-18	-137	-76
-17	-141	30
-16	-136	-60
-15	-139	-151
-14	-135	-33
-13	-134	-34
-12	432	-440
-11	286	-285
-10	291	303
-9	-124	98
-8	373	-364
-7	379	382
-6	-113	32
-5	518	-502
-4	-111	-93
-3	-112	10
-2	185	-200
-1	195	142

H= 8, K= 2

L	FO	FC
0	191	-138
1	-114	4
2	-115	227
3	-116	-121
4	524	-536
5	-121	-108
6	-121	58
7	334	-346
8	363	-370
9	540	539
10	204	202
11	333	-349
12	-133	-37
13	-137	99
14	-136	-105
15	-136	44
16	-146	231
-18	208	221
-17	-140	-31
-16	254	-270
-15	281	267
-14	434	464
-13	393	-438
-12	225	-284
-11	300	305
-10	-129	-121
-9	-125	-240
-8	257	350
-7	-123	-184
-6	587	-613
-5	-114	66
-4	-114	141
-3	-113	-115
-2	-115	116
-1	216	157

H= 8, K= 3

L	FO	FC
0	-115	-72
1	299	309
2	413	412
3	339	-373
4	-122	-113
5	186	-28

L	FO	FC
6	239	228
7	223	173
8	-129	32
9	343	-371
10	320	-311
11	201	82
12	-135	-137
13	-139	-115
14	-137	84
15	-145	160
-17	-145	-128
-16	201	122
-15	-137	100
-14	-135	-42
-13	-135	99
-12	301	320
-11	271	-333
-10	300	-310
-9	412	400
-8	310	292
-7	-122	-47
-6	220	-272
-5	249	-249
-4	-117	-2
-3	-113	85
-2	193	214
-1	-116	-27

H= 8, K= 4

L	FO	FC
0	203	-205
1	-120	-88
2	485	477
3	371	370
4	-128	-93
5	215	-204
6	280	-235
7	307	334
8	558	576
9	357	-361
10	-140	0
11	-132	74
12	-134	-37
13	-137	-34
14	-137	90
15	-146	-244
-17	-144	149
-16	-141	135
-15	-140	-130
-14	-138	-191
-13	420	427
-12	-137	133
-11	320	-371
-10	-129	-85
-9	226	-72
-8	511	531
-7	452	468
-6	433	-428
-5	509	-506
-4	250	-253
-3	366	404
-2	-120	187
-1	-119	-110

H= 8, K= 5

L	FO	FC
0	190	-326
1	449	-449
2	-127	63
3	623	646
4	-131	31
5	247	-230
6	255	-329
7	-135	44
8	-138	94
9	248	215
10	-131	-7
11	-136	-65

L	FO	FC
12	-137	-59
13	351	237
14	-142	3
-16	-138	-84
-15	-138	-13
-14	-129	66
-13	237	-163
-12	-134	69
-11	281	320
-10	-139	-113
-9	229	-150
-8	-136	-7
-7	429	435
-6	-130	200
-5	579	-544
-4	-123	-59
-3	-125	168
-2	198	-94
-1	-129	250
H= 8, K= 6		
0	-132	36
1	-137	-186
2	-134	-76
3	-132	-95
4	-137	72
5	342	344
6	318	-218
7	514	-552
8	426	419
9	393	328
10	313	-344
11	-142	-86
12	-142	212
13	-146	-38
-16	-146	37
-15	-143	135
-14	-138	-103
-13	361	-305
-12	227	152
-11	367	331
-10	214	-1
-9	-141	-122
-8	-136	78
-7	342	-292
-6	196	188
-5	365	334
-4	-136	-146
-3	-133	-17
-2	278	212
-1	-129	76
H= 8, K= 7		
0	410	454
1	486	487
2	453	-460
3	336	-373
4	-143	229
5	-139	111
6	-141	-214
7	-139	177
8	276	223
9	-137	-109
10	-139	-61
11	-141	-39
12	-143	-43
-15	265	-128
-14	233	-132
-13	-143	193
-12	-135	20
-11	-140	-259
-10	-137	99
-9	390	401
-8	304	-305
-7	249	-252
-6	369	375
-5	-139	-108
-4	-136	-170
-3	-134	57
-2	-138	59
-1	-138	-114
H= 8, K= 8		
0	205	106
1	-143	1
2	-141	50
3	-138	65
4	212	-197
5	-139	-154
6	269	325
7	-141	178
8	-141	-174
9	-143	42
10	-148	-21
11	-141	-101
-13	-147	77
-12	-143	-97
-11	-133	-88
-10	219	33
-9	-136	94
-8	-143	210
-7	217	147
-6	419	-453
-5	-140	-231
-4	-145	145
-3	-142	107
-2	-141	13
-1	-147	-100
H= 8, K= 9		
0	387	-393
1	-138	-44
2	-141	202
3	-140	115
4	-138	-45
5	-146	-224
6	-138	38
7	-140	31
8	-147	62
9	-147	-6
10	-151	33
-12	-154	150
-11	-145	-35
-10	-146	-160
-9	-143	0
-8	-141	102
-7	-144	89
-6	-137	-77
-5	-136	20
-4	-138	-12
-3	259	-223
-2	-141	163
-1	-143	160
H= 8, K= 10		
0	-144	-22
1	-138	-85
2	-141	-55
3	-149	127
4	-145	69
5	-146	58
6	307	-263
7	226	-98
-10	-152	-121
-9	268	-232
-8	-142	27
-7	236	162
-6	-144	107
-5	-142	-61
-4	-148	-209
-3	-138	52
-2	-145	136
-1	-138	-46
H= 8, K= 11		
0	-155	201
1	-153	-184
2	316	-276
3	-151	107
4	-153	237
-7	-152	106
-6	-157	235
-5	214	-59
-4	-147	-79
-3	-147	-52
-2	-151	12
-1	-149	133
H= 9, K= 0		
1	-118	-92
3	472	454
5	222	-243
7	325	294
9	267	-256
11	-137	-150
13	395	373
15	500	-493
-17	243	322
-15	224	-211
-13	198	208
-11	-140	-280
-9	-128	32
-7	-126	175
-5	569	-554
-3	-116	107
-1	489	-474
H= 9, K= 1		
0	-119	-157
1	683	-680
2	571	553
3	295	250
4	360	-371
5	-124	-84
6	236	76
7	180	-44
8	-136	3
9	523	523
10	428	-418
11	524	-514
12	287	322
13	354	310
14	-139	-191
15	-142	-134
-17	253	131
-16	-140	-126
-15	-139	101
-14	-130	-24
-13	409	-396
-12	-138	136
-11	613	610
-10	311	-295
-9	-130	-68
-8	334	244
-7	-121	7
-6	226	-253
-5	-118	196
-4	326	309
-3	251	-208
-2	367	-352
-1	335	371
H= 9, K= 2		
0	194	106
1	368	366
2	-124	-15
3	415	-444
4	·264	216
5	-127	93
6	-131	-61
7	-130	-127
8	-135	228
9	-142	189
10	-136	-55
11	-131	29
12	-137	-27
13	275	-244
14	-141	83
15	-151	207
-17	255	-326
-16	377	215
-15	397	423
-14	236	-254
-13	265	-268
-12	-135	132
-11	268	-267
-10	-135	-10
-9	190	194
-8	-128	117
-7	289	-306
-6	-124	158
-5	723	720
-4	447	-425
-3	163	-23
-2	229	226
-1	311	-223
H= 9, K= 3		
0	419	435
1	383	411
2	190	-168
3	-125	-89
4	-123	-30
5	-133	-127
6	-131	34
7	-131	58
8	243	-140
9	-138	-184
10	-142	229
11	265	266
12	-136	-149
13	-138	-93
14	-142	156
-17	-148	87
-16	-140	19
-15	-135	-25
-14	376	367
-13	195	177
-12	483	-443
-11	197	-142
-10	-135	0
-9	-131	-40
-8	-131	63
-7	183	-187
-6	219	59
-5	-125	-74
-4	373	401
-3	240	272
-2	583	-586
-1	203	-205
H= 9, K= 4		
0	-124	-18
1	-123	-8
2	239	221
3	-129	158
4	-129	-42
5	-132	-43
6	-134	168
7	-135	136
8	-143	-171

L	FO	FC
9	579	-591
10	210	-145
11	254	264
12	269	190
13	-144	107
14	-148	-213
-16	391	-298
-15	-136	-56
-14	237	311
-13	212	302
-12	-134	-59
-11	221	-53
-10	-136	-11
-9	-133	2
-8	186	224
-7	-127	62
-6	473	-462
-5	-130	85
-4	252	223
-3	205	78
-2	-122	43
-1	-130	-208
H=	9, K=	5
0	547	-537
1	195	-50
2	683	725
3	-131	137
4	-135	-203
5	-137	133
6	-136	-20
7	-137	178
8	-140	286
9	227	-182
10	261	-305
11	-140	50
12	366	302
13	-148	-102
-16	-146	-38
-15	-139	-81
-14	-137	-132
-13	-139	175
-12	-141	187
-11	-135	-41
-10	-138	-190
-9	-136	29
-8	290	237
-7	-134	118
-6	-130	-17
-5	-133	-174
-4	156	-66
-3	277	317
-2	-124	-105
-1	-130	78
H=	9, K=	6
0	-131	-56
1	-134	76
2	333	-251
3	203	190
4	-139	160
5	-141	-98
6	248	-242
7	-141	178
8	248	286
9	-138	102
10	-143	-134
11	-142	179
12	-145	-79
-15	-146	-62
-14	301	-237
-13	-139	54
-12	-139	116
-11	-133	-3
-10	-138	63
-9	-137	-173

L	FO	FC
-8	-138	-174
-7	-139	153
-6	451	473
-5	208	-205
-4	466	-496
-3	210	258
-2	275	302
-1	361	-368
H=	9, K=	7
0	423	398
1	450	-458
2	325	-327
3	204	206
4	-140	65
5	241	-232
6	-141	161
7	-138	-141
8	-142	-95
9	281	227
10	-144	115
11	249	-155
-14	247	226
-13	-142	-65
-12	-144	-125
-11	-143	32
-10	-135	-55
-9	-138	-46
-8	-136	-104
-7	-137	48
-6	-144	121
-5	-141	-145
-4	362	336
-3	-140	-141
-2	478	-494
-1	216	290
H=	9, K=	8
0	290	-282
1	-143	163
2	-143	175
3	-142	-169
4	239	-200
5	-136	83
6	-139	73
7	-140	-106
8	-141	-126
9	-144	64
10	-141	-2
-12	-143	-34
-11	-150	-85
-10	225	-123
-9	-143	104
-8	-141	172
-7	-138	-118
-6	-140	-205
-5	-142	214
-4	-141	-190
-3	236	-153
-2	462	448
-1	207	-5
H=	9, K=	9
0	252	-261
1	340	352
2	-146	236
3	-146	-123
4	-139	14
5	-144	0
6	-143	23
7	-146	2
8	-149	-98
-11	-148	-133
-10	-141	-54
-9	-142	140

L	FC	FC
-8	-142	149
-7	-143	-24
-6	-144	-180
-5	252	-68
-4	-141	24
-3	299	275
-2	-141	96
-1	366	-366
H=	9, K=	10
0	-140	11
1	-151	-48
2	251	-4
3	292	257
4	-151	-21
5	-147	-104
6	-150	-35
-8	-147	256
-7	-148	196
-6	-142	-76
-5	-147	-142
-4	-148	2
-3	254	164
-2	-140	-15
-1	257	-187
H=	9, K=	11
0	324	-235
1	340	-355
2	284	231
-4	-147	20
-3	-144	-76
-2	-147	88
-1	258	250
H=	10, K=	0
0	-118	121
2	-126	100
4	364	-388
6	472	468
8	378	-353
10	-136	-120
12	368	416
14	486	-469
-16	340	-337
-14	-131	106
-12	-136	130
-10	212	-198
-8	219	253
-6	506	-517
-4	678	681
-2	178	-234
H=	10, K=	1
0	154	-255
1	221	185
2	226	155
3	163	-107
4	-135	73
5	-129	106
6	227	-259
7	-135	73
8	232	314
9	-134	-62
10	299	-271
11	-135	168
12	211	188
13	-142	-189
14	-143	-44
-17	-141	13
-16	275	256
-15	-136	0
-14	-136	-187
-13	-131	-89

L	FO	FC
-12	-137	190
-11	-134	141
-10	-133	-300
-9	-132	99
-8	216	191
-7	368	-392
-6	-134	142
-5	-126	100
-4	597	-611
-3	291	281
-2	678	700
-1	299	-314
H=	10, K=	2
0	494	513
1	-121	5
2	453	-419
3	-131	112
4	156	171
5	293	-281
6	-137	59
7	-136	156
8	-135	-83
9	-136	100
10	-134	59
11	-129	-120
12	218	-249
13	279	234
14	-149	227
-16	-139	170
-15	-138	-102
-14	-132	83
-13	-134	91
-12	-132	32
-11	-136	206
-10	344	319
-9	276	-189
-8	454	-502
-7	203	185
-6	-130	28
-5	-127	-48
-4	-127	196
-3	254	201
-2	274	-219
-1	211	-223
H=	10, K=	3
0	-129	187
1	246	-216
2	233	188
3	-130	-158
4	-128	32
5	-134	254
6	210	291
7	273	-321
8	212	-179
9	-134	119
10	264	271
11	-132	-159
12	-139	-193
13	-141	51
-16	-143	-125
-15	294	266
-14	243	216
-13	201	-240
-12	200	-164
-11	281	356
-10	-137	130
-9	-136	-197
-8	299	294
-7	-133	-111
-6	-129	-79
-5	234	266
-4	223	221
-3	-125	-147
-2	369	-430

L	FO	FC
-1	527	505
H=	10, K=	4
0	272	-235
1	279	252
2	-130	-77
3	-132	19
4	-135	-84
5	-137	224
6	-139	272
7	-136	-54
8	-133	-197
9	-131	-29
10	253	257
11	251	223
12	-138	-25
13	256	-249
-16	229	-96
-15	-143	245
-14	-139	126
-13	-134	48
-12	335	-407
-11	-134	-233
-10	-139	201
-9	-137	195
-8	-137	-10
-7	-136	-250
-6	300	-220
-5	296	234
-4	218	236
-3	204	-227
-2	-130	184
-1	-129	-67
H=	10, K=	5
0	-133	35
1	314	290
2	-134	41
3	273	-178
4	-135	-154
5	-135	-22
6	-136	60
7	-135	178
8	-133	-8
9	332	-310
10	-133	-120
11	271	308
12	-144	86
-15	301	-266
-14	-137	71
-13	-139	189
-12	-133	-12
-11	233	-45
-10	211	-157
-9	-136	138
-8	-138	23
-7	243	-190
-6	-138	-213
-5	226	-199
-4	-135	156
-3	608	641
-2	224	-212
-1	746	-734
H=	10, K=	6
0	-135	63
1	219	-30
2	239	-76
3	-140	34
4	-138	-151
5	217	-274
6	-136	75
7	-137	232
8	-133	43
9	-135	24

L	FO	FC
10	213	-179
11	-142	-235
-14	-141	75
-13	-138	66
-12	-137	94
-11	-134	-113
-10	-135	30
-9	217	-99
-8	192	29
-7	206	222
-6	-136	-90
-5	281	-254
-4	-143	155
-3	-134	71
-2	288	-286
-1	-139	188
H=	10, K=	7
0	461	-478
1	-128	-38
2	336	360
3	-135	-172
4	-131	-41
5	211	174
6	-138	-212
7	245	-220
8	-141	246
9	234	239
10	313	-238
-13	217	-190
-12	-137	43
-11	-134	141
-10	235	-67
-9	-131	134
-8	-128	115
-7	-135	-253
-6	-127	24
-5	191	13
-4	-128	60
-3	-137	-295
-2	281	283
-1	380	345
H=	10, K=	8
0	-139	140
1	379	435
2	272	-248
3	-138	-79
4	-136	88
5	-135	-22
6	-134	104
7	-141	-148
8	-145	9
9	-143	81
-11	-142	-58
-10	-135	114
-9	213	180
-8	220	-231
-7	-136	-124
-6	-138	75
-5	-138	200
-4	-136	-48
-3	-136	57
-2	-140	122
-1	560	-591
H=	10, K=	9
0	273	169
1	-143	-67
2	-146	-63
3	-138	14
4	-148	-130
5	207	-10
6	-152	184
7	-148	134

L	FO	FC
-9	-147	62
-8	-142	70
-7	-140	-94
-6	-144	-150
-5	-144	71
-4	-144	162
-3	243	53
-2	-145	-268
-1	-137	59
H=	10, K=	10
0	-146	-46
1	-150	63
2	-144	112
3	-146	-40
4	-147	-56
-6	-155	-222
-5	-145	-2
-4	220	240
-3	-145	45
-2	234	-103
-1	-150	-51
H=	11, K=	0
1	609	633
3	298	-354
5	378	395
7	-132	-54
9	246	243
11	193	132
13	534	-476
-15	-141	124
-13	-133	-88
-11	-129	28
-9	438	426
-7	-130	-38
-5	-126	130
-3	-124	-26
-1	652	-661
H=	11, K=	1
0	619	637
1	-130	140
2	-131	-183
3	-129	11
4	-129	20
5	409	-420
6	-134	64
7	297	253
8	-137	-161
9	-133	62
10	-135	131
11	-138	131
12	-135	-82
13	-144	143
-16	-145	-6
-15	272	-307
-14	-139	97
-13	-137	74
-12	-135	-97
-11	-135	52
-10	214	210
-9	-135	-74
-8	-132	58
-7	158	226
-6	-130	177
-5	-133	-211
-4	-131	-229
-3	750	750
-2	230	-230
-1	504	-531
H=	11, K=	2
0	-133	-165

L	FO	FC
1	315	-331
2	286	227
3	207	235
4	-132	-104
5	-137	-112
6	-134	165
7	-135	-102
8	-133	23
9	-134	38
10	-136	-1
11	-139	-137
12	-141	160
13	310	293
-16	-145	-147
-15	-139	-6
-14	-138	70
-13	-137	-168
-12	-132	-132
-11	-137	44
-10	-136	-17
-9	340	-312
-8	373	295
-7	232	282
-6	-133	-196
-5	226	-59
-4	-130	78
-3	433	-476
-2	230	159
-1	904	890
H=	11, K=	3
0	-129	-92
1	-132	44
2	206	-202
3	199	1
4	259	292
5	287	250
6	245	-192
7	208	-160
8	-131	71
9	-136	-17
10	-137	48
11	-138	-48
12	-138	-8
-15	238	234
-14	264	-278
-13	-135	-113
-12	-137	-132
-11	234	183
-10	-135	108
-9	-137	-132
-8	-136	-185
-7	-135	-189
-6	-129	84
-5	-129	75
-4	466	-470
-3	-131	-101
-2	515	555
-1	-136	-228
H=	11, K=	4
0	311	337
1	293	250
2	340	-318
3	358	-340
4	336	245
5	-135	102
6	-132	-46
7	-130	-43
8	-134	-65
9	199	57
10	-137	46
11	-135	-83
12	266	-252
-15	-140	-8
-14	-143	7

L	FO	FC
-13	203	-105
-12	-131	-75
-11	-132	128
-10	347	365
-9	-131	-11
-8	335	-375
-7	-135	66
-6	-134	-17
-5	199	179
-4	-133	50
-3	-137	-197
-2	365	-394
-1	-136	-193

H= 11, K= 5

L	FO	FC
0	421	372
1	-136	-110
2	-138	-116
3	269	-250
4	-139	-125
5	-136	127
6	-136	178
7	-133	88
8	-138	-184
9	-142	-53
10	-147	158
11	274	107
-14	234	170
-13	-143	-5
-12	253	-219
-11	-137	-137
-10	-138	192
-9	-137	172
-8	-140	63
-7	-134	-105
-6	-133	55
-5	-132	-5
-4	-134	159
-3	-137	-3
-2	698	-668
-1	431	426

H= 11, K= 6

L	FO	FC
0	548	-523
1	262	249
2	363	354
3	-139	-86
4	314	-336
5	-136	9
6	-138	195
7	225	-96
8	-140	-53
9	-143	-51
10	-149	6
-13	-142	-103
-12	-143	63
-11	-135	-3
-10	-136	-58
-9	-138	80
-8	-134	35
-7	-135	-67
-6	211	-131
-5	-131	-41
-4	-136	179
-3	-138	-128
-2	326	291
-1	-137	-53

H= 11, K= 7

L	FO	FC
0	253	256
1	-137	170
2	290	-300
3	-139	5
4	-137	145
5	-140	-124
6	320	-248
7	227	227
8	-149	112
9	243	-167
-12	-143	78
-11	-144	-25
-10	-143	23
-9	-140	22
-8	-137	-138
-7	-137	-47
-6	238	228
-5	-137	5
-4	228	-184
-3	-136	-3
-2	-140	33
-1	-140	-207

H= 11, K= 8

L	FO	FC
0	239	210
1	-141	-154
2	-144	-116
3	-144	24
4	-145	113
5	-143	-39
6	-149	120
7	-148	-58
-10	-145	97
-9	226	-120
-8	-146	-124
-7	264	194
-6	-138	-25
-5	-138	-64
-4	-142	91
-3	-140	-75
-2	-141	-69
-1	-140	125

H= 11, K= 9

L	FO	FC
0	-145	-104
1	-142	-48
2	-146	123
3	-146	-97
4	-148	-61
-7	-149	-154
-6	-146	-22
-5	242	228
-4	-141	-15
-3	214	-151
-2	-143	-29
-1	-144	190

H= 12, K= 0

L	FO	FC
0	947	991
2	-133	-134
4	-138	333
6	250	-218
8	-137	3
10	-143	186
12	294	-357
-14	-135	43
-12	199	137
-10	-128	-1
-8	-135	-158
-6	-131	59
-4	380	369
-2	1112	-1095

H= 12, K= 1

L	FO	FC
0	-130	104
1	-131	-62
2	-131	49
3	249	207
4	-136	-161
5	-136	112
6	240	242
7	-133	-67
8	164	10
9	-143	145
10	-137	-36
11	-141	-34
-15	-135	62
-14	-141	65
-13	-133	22
-12	-138	-24
-11	-138	86
-10	-132	-111
-9	264	-278
-8	240	247
-7	-133	71
-6	260	-222
-5	-140	175
-4	341	258
-3	-134	-151
-2	622	-650
-1	-131	5

H= 12, K= 2

L	FO	FC
0	835	-824
1	-139	227
2	-132	40
3	-134	-173
4	-139	169
5	-131	34
6	191	-155
7	-136	-44
8	-136	107
9	-134	0
10	-145	-106
11	270	208
-15	-142	-33
-14	-142	-144
-13	-139	5
-12	-137	118
-11	-134	-6
-10	-133	-83
-9	-133	11
-8	-134	-86
-7	-134	-91
-6	-134	153
-5	-130	2
-4	218	-167
-3	-134	49
-2	808	817
-1	557	-551

H= 12, K= 3

L	FO	FC
0	-138	139
1	212	-179
2	-141	-79
3	-136	-30
4	-135	57
5	-137	-101
6	-133	-41
7	192	40
8	-130	-61
9	-135	-9
10	-139	16
11	-146	-162
-14	-144	-119
-13	202	173
-12	-134	3
-11	-138	-6
-10	-129	78
-9	309	-273
-8	-139	-153
-7	317	337
-6	-137	174
-5	-136	-207
-4	350	-261
-3	421	423
-2	-135	148
-1	-137	-214

H= 12, K= 4

L	FO	FC
0	-136	-58
1	546	-508
2	-135	13
3	-135	77
4	-134	215
5	-131	-6
6	-132	-50
7	-136	-32
8	220	-54
9	-135	5
10	-142	142
-14	-145	17
-13	267	-86
-12	-139	40
-11	-139	100
-10	-137	-75
-9	-136	-193
-8	305	-228
-7	-134	47
-6	311	270
-5	-139	214
-4	-140	-208
-3	408	-449
-2	-138	-41
-1	794	810

H= 12, K= 5

L	FO	FC
0	225	161
1	-134	72
2	-137	-190
3	-135	-69
4	-131	45
5	-137	176
6	-142	-95
7	279	-250
8	-137	46
9	-150	112
-13	-149	19
-12	-141	0
-11	-136	-39
-10	201	107
-9	-136	-1
-8	219	-85
-7	-136	-166
-6	-136	128
-5	-136	222
-4	-138	-10
-3	271	-337
-2	369	-351
-1	356	257

H= 12, K= 6

L	FO	FC
0	-135	-72
1	350	397
2	-135	-126
3	207	-195
4	-138	141
5	-141	30
6	289	-159
7	-147	118
8	-148	-68
-12	-143	-10
-11	-139	-61
-10	-140	11
-9	214	208
-8	206	-123
-7	-139	0
-6	-145	205
-5	-134	-154
-4	-134	32
-3	-137	36

L	FO	FC
-2	192	73
-1	304	-263
H=	12, K=	7
0	193	128
1	200	-196
2	-143	127
3	205	135
4	-142	-67
5	-143	-48
6	-146	141
7	-140	-16
-10	-144	7
-9	-147	-184
-8	-140	17
-7	209	270
-6	-140	-100
-5	-143	-109
-4	-139	144
-3	201	164
-2	-134	-102
-1	-137	-72
H=	12, K=	8
0	298	-195
1	232	-135
2	-147	63
3	-141	28
4	-144	-42
5	-150	171
-8	254	143
-7	-144	-108
-6	-143	28
-5	-140	144
-4	-144	-194
-3	275	-102
-2	-148	195
-1	253	184
H=	12, K=	9
0	-151	55
1	-145	-74
-4	-151	-90
-3	-144	-90
-2	-150	28
-1	-146	81

L	FO	FC
H=	13, K=	0
1	-136	-86
3	202	98
5	-135	167
7	207	-190
9	212	160
-13	-140	32
-11	-136	38
-9	-134	-106
-7	-134	0
-5	-138	36
-3	683	-674
-1	430	442
H=	13, K=	1
0	-132	-139
1	-133	117
2	-130	65
3	285	-284
4	-135	19
5	298	294
6	-138	-179
7	-135	-128
8	209	111
9	-138	24
10	-146	-37
-14	-146	-83
-13	-139	55
-12	-139	106
-11	-136	-195
-10	-133	-16
-9	266	298
-8	-130	-8
-7	-130	-116
-6	-132	-2
-5	271	169
-4	218	-310
-3	258	-257
-2	220	270
-1	277	-156
H=	13, K=	2
0	210	78
1	226	-193
2	-131	-64
3	-136	29
4	-132	89

L	FO	FC
5	-134	-177
6	-139	-16
7	259	292
8	-138	-51
9	223	-158
10	-143	46
-13	-138	116
-12	-143	-126
-11	198	-166
-10	-133	187
-9	-138	99
-8	-136	-150
-7	-134	99
-6	-136	39
-5	390	-370
-4	223	143
-3	505	552
-2	344	-286
-1	-138	-173
H=	13, K=	3
0	202	-223
1	-133	-117
2	-137	150
3	-136	29
4	298	-249
5	-134	-74
6	213	246
7	-140	-160
8	-141	65
9	-144	64
-13	-138	-33
-12	-139	123
-11	-141	109
-10	-139	-137
-9	383	-289
-8	-135	210
-7	-132	182
-6	240	-274
-5	410	-417
-4	-135	69
-3	547	525
-2	-143	273
-1	-136	-252
H=	13, K=	4
0	210	-248
1	-136	-15

L	FO	FC
2	-135	-41
3	-140	-20
4	'195	124
5	230	-13
6	-141	-206
7	-141	-77
8	-144	125
9	-143	46
-12	-145	100
-11	-140	44
-10	-140	-153
-9	264	204
-8	-136	70
-7	194	-20
-6	-133	154
-5	-140	-245
-4	400	-404
-3	230	106
-2	406	428
-1	268	195
H=	13, K=	5
0	-135	-99
1	-139	-143
2	-138	54
3	-138	153
4	240	228
5	-138	-80
6	290	-298
7	-143	111
8	257	99
-11	-142	-12
-10	-141	149
-9	-140	66
-8	-143	-264
-7	-142	60
-6	318	293
-5	-134	121
-4	241	-221
-3	-138	-207
-2	-135	140
-1	315	287
H=	13, K=	6
-10	-142	16
-9	-141	-123
-8	-143	39

Table B-2

Observed and Calculated Structure Factors for [Co(Hdmg)$_2$-(clan)$_2$]Cℓ

L	FO	FC
H=	0, K=	0
1	765	730
2	469	420
3	137	121
4	202	177
5	437	405
6	48	35
7	357	342
8	75	73
9	229	219
10	55	58
11	230	229
12	103	108
13	43	39
H=	0, Y=	1
0	651	638
1	426	400
2	345	309
3	177	164
4	235	-217
5	172	161
6	315	-270
7	226	191
8	101	105
9	66	54
10	190	193
11	81	83
12	174	177
13	27	21
-13	53	57
-12	44	-48
-11	101	103
-10	-14	15
-9	67	-62
-8	-12	-8
-7	31	1
-6	555	519
-5	231	216
-4	349	337
-3	103	-103
-2	84	-73
-1	443	431
H=	0, K=	2
0	475	-471
1	394	367
2	299	279
3	209	188
4	146	131
5	40	-36
6	487	464
7	269	256
8	320	303
9	115	114
10	297	291
11	74	78
12	91	87
-13	34	38
-12	52	47
-11	36	38
-10	102	103
-9	-14	21
-8	238	241
-7	67	73
-6	486	472
-5	547	512
-4	476	450
-3	458	450
-2	235	228
-1	673	668
H=	0, K=	3
0	155	-142
1	134	-126
2	40	35
3	95	-88
4	28	30
5	118	-113
6	295	270
7	140	137
8	135	131
9	184	184
10	60	61
11	95	95
12	-12	-10
-12	68	69
-11	-12	-16
-10	42	-44
-9	135	133
-8	117	117
-7	116	113
-6	15	23
-5	234	238
-4	173	163
-3	41	29
-2	304	-292
-1	239	-225
H=	0, K=	4
0	211	199
1	194	191
2	333	332
3	235	224
4	202	201
5	328	329
6	132	131
7	204	199
8	68	67
9	138	136
10	60	58
11	132	137
-12	104	107
-11	104	105
-10	146	147
-9	224	230
-8	75	78
-7	194	190
-6	160	155
-5	210	214
-4	283	285
-3	31	30
-2	21	19
-1	112	-102
H=	0, K=	5
0	-10	8
1	271	266
2	193	190
3	89	94
4	58	54
5	138	140
6	93	91
7	21	28
8	59	-61
9	51	-49
10	28	26
-11	92	94
-10	195	196
-9	90	93
-8	16	-9
-7	20	-16
-6	61	60
-5	60	53
-4	34	-30
-3	73	-72
-2	36	42
-1	25	-19
H=	0, K=	6
0	262	263
1	371	379
2	299	295
3	247	258
4	195	197
5	128	131
6	172	172
7	43	44
8	70	74
9	68	63
-10	131	136
-9	92	91
-8	101	99
-7	75	70
-6	140	141
-5	206	204
-4	178	178
-3	228	228
-2	190	188
-1	185	189
H=	0, K=	7
0	76	78
1	27	28
2	59	58
3	124	123
4	97	100
5	54	48
6	-11	0
7	32	37
8	110	112
-9	-12	2
-8	-11	10
-7	-11	-2
-6	-11	-7
-5	69	68
-4	214	211
-3	242	247
-2	126	128
-1	61	64
H=	0, K=	8
0	104	111
1	67	66
2	93	99
3	111	112
4	103	106
5	54	57
6	90	90
-7	83	83
-6	51	52
-5	79	78
-4	193	194
-3	280	282
-2	273	276
-1	192	193
H=	0, K=	9
0	-11	5
1	-11	17
2	26	30
-3	26	24
-2	45	45
-1	26	29
H=	1, K=	0
0	699	676
1	250	242
2	45	40
3	671	651
4	337	324
5	520	491
6	15	-6
7	238	230
8	241	254
9	64	62
10	229	234
11	126	131
12	197	199
-13	122	128
-12	42	41
-11	147	155
-10	195	194
-9	111	110
-8	365	367
-7	231	223
-6	414	384
-5	24	25
-4	311	300
-3	30	-21
-2	43	45
-1	653	627
H=	1, K=	1
0	238	-229
1	99	94
2	315	-301
3	110	-115
4	343	330
5	72	-61
6	223	217
7	34	32
8	287	281
9	-11	11
10	127	127
11	17	32
12	-12	-4
-13	-12	14
-12	60	60
-11	100	99
-10	144	148
-9	175	-173
-8	166	177
-7	55	53
-6	88	69
-5	164	-164
-4	399	-370
-3	285	292
-2	176	-174
-1	426	421
H=	1, K=	2
0	413	394
1	59	53
2	411	392
3	81	85
4	284	260
5	37	38
6	241	225
7	194	188
8	213	204
9	322	323
10	81	79
11	70	72
12	78	-78
-13	74	74
-12	145	151
-11	110	113
-10	28	-27
-9	146	144
-8	126	132
-7	269	266
-6	140	143
-5	159	160
-4	44	-37
-3	306	323
-2	300	296
-1	302	284

L	FO	FC
H=	1, K=	3
0	156	159
1	237	-231
2	146	140
3	247	239
4	33	37
5	130	127
6	146	-142
7	157	150
8	-11	-12
9	129	123
10	66	68
11	-11	9
-13	96	99
-12	101	102
-11	-11	10
-10	108	-109
-9	133	137
-8	50	47
-7	96	96
-6	-10	15
-5	29	28
-4	257	249
-3	131	-132
-2	186	178
-1	183	177
H=	1, K=	4
0	298	295
1	405	400
2	233	230
3	294	284
4	246	244
5	208	203
6	142	136
7	113	110
8	28	24
9	25	22
10	148	151
-12	63	86
-11	65	64
-10	128	127
-9	127	127
-8	228	232
-7	266	267
-6	263	291
-5	254	251
-4	231	240
-3	114	117
-2	320	319
-1	495	489
H=	1, K=	5
0	152	140
1	314	313
2	136	135
3	39	44
4	135	133
5	95	94
6	183	179
7	99	-105
8	46	-44
9	56	54
-11	38	27
-10	71	76
-9	-11	0
-8	55	53
-7	179	175
-6	298	302
-5	244	241
-4	20	-11
-3	-9	14
-2	13	4
-1	67	76

L	FO	FC
H=	1, K=	6
0	221	225
1	184	182
2	166	166
3	176	172
4	188	177
5	244	233
6	144	151
7	37	34
8	102	104
-10	105	104
-9	72	69
-8	30	28
-7	113	110
-6	260	252
-5	309	314
-4	246	240
-3	176	175
-2	160	158
-1	152	153
H=	1, K=	7
0	53	59
1	16	-14
2	-11	-5
3	47	47
4	52	52
5	56	58
6	-12	0
7	98	101
-9	-12	15
-8	-12	-17
-7	30	-28
-6	22	-20
-5	36	35
-4	79	80
-3	68	64
-2	62	82
-1	77	75
H=	1, K=	8
0	95	98
1	114	116
2	114	115
3	104	107
4	100	98
-7	82	80
-6	63	63
-5	54	52
-4	84	87
-3	149	145
-2	119	122
-1	82	83
H=	1, K=	-9
0	66	68
1	118	119
2	84	83
3	21	15
-3	36	33
-2	34	37
-1	25	24
H=	1, K=	-8
0	109	110
1	147	154
2	174	177
3	180	186
4	138	139
5	100	101
6	122	123
7	131	131

L	FO	FC
-6	127	135
-5	175	175
-4	193	187
-3	166	173
-2	104	107
-1	63	65
H=	1, K=	-7
0	22	24
1	30	33
2	63	63
3	107	107
4	33	29
5	16	-12
6	38	42
7	100	102
8	99	104
-8	93	93
-7	41	42
-6	40	35
-5	36	35
-4	92	86
-3	45	48
-2	46	-47
-1	22	-11
H=	1, K=	-6
0	134	141
1	229	225
2	242	248
3	165	165
4	124	127
5	120	118
6	99	101
7	113	114
8	112	111
9	82	86
10	134	136
-10	113	112
-9	83	85
-8	97	94
-7	121	123
-6	78	72
-5	114	117
-4	141	141
-3	129	125
-2	73	70
-1	75	76
H=	1, K=	-5
0	99	98
1	55	55
2	145	143
3	15	17
4	-10	3
5	62	61
6	40	38
7	28	32
8	37	-42
9	68	66
10	77	79
11	37	40
-11	116	124
-10	48	44
-9	71	68
-8	-11	-7
-7	41	-41
-6	75	-68
-5	72	69
-4	-10	-2
-3	17	-15
-2	18	11
-1	48	-51
H=	1, K=	-4

L	FO	FC
0	244	232
1	168	166
2	395	384
3	437	427
4	184	186
5	116	119
6	103	105
7	177	181
8	111	113
9	126	117
10	75	68
11	27	26
-12	105	109
-11	114	115
-10	71	75
-9	170	168
-8	133	134
-7	-11	-2
-6	262	251
-5	245	229
-4	350	334
-3	214	207
-2	194	193
-1	381	380
H=	1, K=	-3
0	629	-617
1	71	66
2	198	192
3	375	361
4	314	297
5	59	-53
6	70	67
7	36	36
8	159	162
9	-11	3
10	-11	-9
11	-11	-19
12	28	25
-12	62	62
-11	18	-21
-10	102	105
-9	-11	-12
-8	79	82
-7	40	36
-6	231	219
-5	106	103
-4	439	421
-3	542	507
-2	289	268
-1	265	261
H=	1, K=	-2
0	106	-102
1	411	392
2	346	328
3	163	164
4	503	452
5	283	270
6	405	396
7	118	116
8	191	189
9	204	204
10	31	29
11	76	73
12	41	45
-13	35	35
-12	106	108
-11	57	57
-10	206	201
-9	254	245
-8	197	193
-7	436	404
-6	23	26
-5	312	291

L	FO	FC
-4	421	384
-3	1149	1097
-2	1301	1250
-1	189	167
H=	1, K=	-1
0	874	852
1	67	-60
2	120	110
3	112	112
4	85	-71
5	406	383
6	19	23
7	130	135
8	-10	20
9	225	222
10	46	45
11	105	104
12	87	92
-13	43	40
-12	18	-6
-11	62	61
-10	19	24
-9	359	359
-8	186	176
-7	316	302
-6	88	-88
-5	45	-38
-4	47	-52
-3	18	3
-2	734	686
-1	166	-177
H=	2, K=	0
0	264	232
1	495	467
2	301	285
3	196	184
4	423	413
5	119	120
6	438	444
7	93	97
8	121	121
9	108	-110
10	-11	-6
11	85	92
-13	48	48
-12	79	84
-11	119	122
-10	329	329
-9	35	33
-8	193	195
-7	18	-4
-6	22	13
-5	272	256
-4	94	-85
-3	368	350
-2	66	58
-1	534	524
H=	2, K=	1
0	648	637
1	188	176
2	201	194
3	170	-150
4	24	-18
5	101	-98
6	22	-21
7	82	83
8	48	46
9	78	82
10	116	-117
11	56	56
-13	-12	-9
-12	40	43

L	FO	FC
-11	177	178
-10	-12	8
-9	42	44
-8	48	-42
-7	97	102
-6	87	-85
-5	24	-14
-4	56	52
-3	395	384
-2	96	88
-1	94	-84
H=	2, K=	2
0	441	445
1	172	181
2	282	275
3	244	238
4	107	-100
5	147	153
6	180	-177
7	271	266
8	187	189
9	164	159
10	80	85
-13	98	103
-12	76	82
-11	163	167
-10	77	80
-9	265	269
-8	141	147
-7	184	178
-6	176	182
-5	88	95
-4	679	670
-3	581	564
-2	672	646
-1	319	301
H=	2, K=	3
0	108	-108
1	71	72
2	103	100
3	156	152
4	43	-38
5	120	-123
6	32	36
7	221	217
8	185	186
9	47	47
10	152	156
-12	-12	6
-11	47	-49
-10	82	78
-9	199	197
-8	304	310
-7	108	109
-6	56	64
-5	63	65
-4	203	201
-3	192	192
-2	269	266
-1	385	374
H=	2, K=	4
0	92	96
1	258	254
2	308	306
3	231	237
4	283	282
5	48	47
6	340	332
7	168	169
8	142	146
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L	FO	FC
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3	172	174
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L	FO	FC
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L	FO	FC
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H=	5, K=	-4
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2	129	126
3	57	62

L	FO	FC
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-5	110	110
-4	44	45
-3	16	3
-2	43	38
-1	155	157
H=	5, K=	-2
0	246	248
1	270	265
2	224	233
3	202	197
4	60	66
5	54	52
6	136	144
-11	71	75
-10	-12	25
-9	98	98
-8	111	110
-7	134	134
-6	157	160

L	FU	FC
-5	218	221
-4	307	308
-3	223	225
-2	218	219
-1	165	165
H=	5, K=	-1
0	128	132
1	215	213
2	73	71
3	75	77
4	21	-30
5	140	145
6	104	102
-11	-12	5
-10	20	17
-9	25	25
-8	-11	15
-7	25	18
-6	91	92
-5	114	116
-4	257	254
-3	139	140
-2	127	127
-1	84	85
H=	6, K=	0
0	111	116
1	35	36
2	105	108
3	95	94
-9	64	63
-8	80	82
-7	151	147
-6	216	222
-5	238	235
-4	33	-33
-3	52	-55
-2	20	19
-1	44	43
H=	6, K=	1
0	40	37
1	29	30
2	86	92
-8	-11	-9

L	FO	FC
-7	23	25
-6	146	153
-5	70	67
-4	17	1
-3	23	-27
-2	-11	6
-1	35	33
H=	6, K=	2
0	127	127
1	216	219
-7	80	85
-6	120	116
-5	73	76
-4	149	148
-3	127	131
-2	104	102
-1	148	149
H=	6, K=	3
-5	84	85
-4	100	100
-3	142	137
-2	94	95
H=	6, K=	-5
0	98	100
-6	44	46
-5	-11	8
-4	26	20
-3	54	52
-2	57	57
-1	95	94
H=	6, K=	-4
0	185	186
1	139	139
2	115	117
-8	126	128
-7	160	165
-6	140	147
-5	101	104
-4	69	72
-3	133	134
-2	182	185

L	FO	FC
-1	210	215
H=	6, K=	-3
0	80	83
1	67	65
2	74	78
3	97	96
-9	32	29
-8	42	47
-7	70	71
-6	88	91
-5	40	43
-4	82	83
-3	130	130
-2	176	176
-1	147	147
H=	6, K=	-2
0	126	130
1	93	92
2	31	29
3	78	79
-9	98	97
-8	135	135
-7	116	122
-6	61	61
-5	49	55
-4	206	203
-3	183	184
-2	189	194
-1	201	204
H=	6, K=	-1
0	94	92
1	39	39
2	28	-32
3	17	-16
-9	50	51
-8	115	113
-7	111	114
-6	20	17
-5	65	66
-4	-11	-11
-3	45	-49
-2	15	2

Table B-3

Observed and Calculated Structure Factors for H_2dhphpy$(NO_3)_2 \cdot 2H_2O$

L	FO	FC
H= 0, K= 0		
2	321	323
4	105	-108
6	292	283
8	247	-242
10	37	-25
H= 2, K= 0		
0	334	342
2	247	-241
4	256	222
6	26	22
8	96	-95
10	73	77
H= 4, K= 0		
0	361	-397
2	2484	-2599
4	135	128
6	26	35
8	169	-163
10	89	100
H= 6, K= 0		
0	850	840
2	531	-525
4	131	126
6	-18	-30
8	58	-55
10	-22	14
H= 8, K= 0		
0	296	-299
2	62	-69
4	963	997
6	60	53
8	40	43
H= 10, K= 0		
0	54	41
2	324	-325
4	239	229
6	46	-45
8	-21	10
H= 12, K= 0		
0	89	-89
2	67	76
4	-20	23
6	390	-402
8	56	-54
H= 14, K= 0		
0	-18	5
2	-19	1
4	222	233
6	79	-87
H= 16, K= 0		
0	158	-152
2	-21	-7
4	-21	5
H= 18, K= 0		
0	157	-163
2	51	-44
4	-22	-8

L	FO	FC
H= 20, K= 0		
0	32	25
2	82	85
H= -22, K= 0		
2	40	22
H= -20, K= 0		
2	38	47
4	88	-83
6	-23	42
H= -18, K= 0		
2	36	40
4	45	-54
6	-22	1
8	148	-147
H= -16, K= 0		
2	30	-21
4	30	-40
6	134	138
8	110	-104
H= -14, K= 0		
2	265	266
4	-20	-3
6	65	66
8	-21	-23
10	101	108
H= -12, K= 0		
2	234	221
4	194	192
6	88	85
8	112	-121
10	78	84
H= -10, K= 0		
2	30	-32
4	585	-543
6	-18	-5
8	49	-46
10	42	48
H= -8, K= 0		
2	404	382
4	523	-523
6	317	-335
8	-20	-12
10	118	118
H= -6, K= 0		
2	431	439
4	267	273
6	445	395
8	42	-35
10	44	41
H= -4, K= 0		
2	196	184
4	587	-581
6	523	524
8	103	97
10	35	-24

L	FO	FC
H= -2, K= 0		
2	1071	-1111
4	343	-334
6	98	95
8	97	-98
10	-21	-5
H= 1, K= 1		
0	401	-389
1	354	-325
2	77	-84
3	135	-133
4	159	-157
5	120	123
6	68	-76
7	47	-49
8	29	17
9	-20	-18
10	-20	18
11	-21	-4
H= 3, K= 1		
0	113	-105
1	419	-425
2	453	441
3	469	455
4	165	170
5	206	207
6	113	115
7	163	163
8	-19	-14
9	90	89
10	61	-60
H= 5, K= 1		
0	549	551
1	969	-986
2	499	493
3	107	-106
4	233	228
5	97	90
6	110	117
7	47	-52
8	-20	23
9	40	42
10	44	-27
H= 7, K= 1		
0	72	75
1	65	55
2	226	-229
3	94	102
4	309	-300
5	213	-217
6	54	-55
7	52	-60
8	46	-51
9	-21	-17
H= 9, K= 1		
0	111	-111
1	23	30
2	153	-174
3	662	661
4	244	-250
5	30	-24
6	76	-76
7	72	-72
8	32	-40
9	40	35
H= 11, K= 1		

L	FO	FC
0	118	115
1	126	-130
2	-18	-4
3	-18	22
4	62	84
5	37	-50
6	100	97
7	40	56
8	-22	11
H= 13, K= 1		
0	88	-97
1	128	-137
2	-19	-10
3	-19	15
4	39	41
5	239	-253
6	117	114
7	32	30
H= 15, K= 1		
0	35	-27
1	-20	37
2	-20	-16
3	53	59
4	-21	7
5	-22	-27
6	-22	-18
H= 17, K= 1		
0	113	114
1	133	131
2	-21	23
3	-22	21
4	-22	11
5	-22	-19
H= 19, K= 1		
0	-21	2
1	-21	12
2	-22	1
3	-22	-9
H= 21, K= 1		
0	-22	-20
H= -21, K= 1		
1	-23	-17
2	-22	-22
3	-22	-4
4	-23	-28
5	-23	22
H= -19, K= 1		
1	87	83
2	-21	-3
3	47	43
4	42	52
5	-22	-11
6	-22	-15
7	68	-70
H= -17, K= 1		
1	111	111
2	64	58
3	47	50
4	65	62
5	38	28
6	31	39

L	FO	FC
7	-22	-34
8	-23	29
9	39	-34
H= -15, K=		1
1	-19	-17
2	-19	20
3	149	-140
4	40	-29
5	57	-58
6	56	-60
7	33	32
8	-21	12
9	36	52
H= -13, K=		1
1	295	284
2	216	-214
3	232	-236
4	55	-58
5	-20	-4
6	83	-90
7	34	-12
8	-21	-22
9	58	71
10	42	-41
H= -11, K=		1
1	128	133
2	27	27
3	91	-67
4	43	-35
5	71	68
6	79	88
7	42	40
8	56	51
9	-21	3
10	-21	0
11	-22	-10
H= -9, K=		1
1	334	-330
2	129	122
3	306	-301
4	115	107
5	187	176
6	38	37
7	71	-71
8	73	74
9	-21	24
10	-21	26
11	-23	-43
H= -7, K=		1
1	81	-54
2	86	-82
3	96	101
4	162	154
5	275	268
6	-17	12
7	88	-89
8	-20	-34
9	51	-49
10	36	-31
11	-22	-24
H= -5, K=		1
1	332	-332
2	315	314
3	264	250
4	64	-49
5	323	314

L	FO	FC
6	133	-123
7	31	-26
8	99	-93
9	32	9
10	49	-47
11	52	-45
H= -3, K=		1
1	125	141
2	202	-206
3	181	-161
4	45	-51
5	106	-119
6	80	-71
7	-18	-18
8	-19	-5
9	87	86
10	-20	0
11	-22	2
H= -1, K=		1
1	397	-422
2	413	-414
3	115	111
4	149	-148
5	348	-345
6	51	60
7	284	-283
8	145	145
9	-21	32
10	46	47
11	-22	16
H= 0, K=		2
0	431	-441
1	510	498
2	93	94
3	322	325
4	282	291
5	149	147
6	63	-59
7	-18	-22
8	51	-43
9	104	-105
10	38	-38
11	43	-43
H= 2, K=		2
0	178	153
1	720	-716
2	313	-311
3	226	231
4	33	-44
5	117	133
6	80	-81
7	50	-55
8	-20	-6
9	-20	-14
10	-20	2
H= 4, K=		2
0	127	126
1	404	394
2	128	131
3	159	-162
4	186	-161
5	45	-56
6	85	-86
7	64	-58
8	74	76
9	34	-27
10	-21	24

L	FO	FC
H= 6, K=		2
0	181	183
1	-15	-1
2	69	-66
3	61	-55
4	65	59
5	152	-154
6	64	-59
7	-20	-18
8	-20	24
9	-21	21
H= 8, K=		2
0	163	164
1	187	-181
2	-16	2
3	104	-117
4	-17	3
5	58	63
6	53	55
7	-21	37
8	-20	9
9	-22	30
H= 10, K=		2
0	114	112
1	79	86
2	-17	-9
3	29	-20
4	106	108
5	30	14
6	-21	19
7	-21	13
8	31	30
H= 12, K=		2
0	140	133
1	-18	8
2	128	-139
3	81	80
4	-20	-24
5	96	100
6	29	2
7	-21	-26
H= 14, K=		2
0	65	-62
1	55	56
2	58	-56
3	-20	10
4	66	-56
5	45	46
6	47	-39
H= 16, K=		2
0	40	-51
1	-20	-24
2	38	-24
3	36	-18
4	54	46
5	52	-47
H= 18, K=		2
0	-21	-24
1	-21	-3
2	31	31
3	-22	-5
4	-23	16
H= 20, K=		2

L	FO	FC
0	-22	3
1	37	-31
2	-23	16
H= -20, K=		2
1	49	45
2	46	45
3	-22	-18
4	37	-11
5	73	-70
6	-23	20
H= -18, K=		2
1	34	-42
2	-21	8
3	62	52
4	31	-36
5	93	87
6	46	-55
7	-22	7
8	-23	-3
H= -16, K=		2
1	119	-108
2	-20	-24
3	69	-74
4	110	-107
5	37	15
6	40	26
7	112	110
8	-22	-14
9	39	38
H= -14, K=		2
1	53	-61
2	52	52
3	69	66
4	101	-102
5	70	-72
6	-21	35
7	80	-86
8	91	93
9	32	19
10	-23	9
H= -12, K=		2
1	66	58
2	175	176
3	154	155
4	-19	12
5	103	100
6	109	109
7	-20	-2
8	-21	-26
9	80	-81
10	-22	36
H= -10, K=		2
1	150	151
2	159	162
3	73	70
4	39	-43
5	224	-225
6	125	134
7	71	75
8	91	-95
9	50	56
10	83	-84
11	-23	8

L	FO	FC
H= -8, K= 2		
1	173	174
2	313	-313
3	141	138
4	121	-106
5	77	-77
6	69	67
7	117	-122
8	103	-105
9	-21	-5
10	-21	-21
11	38	46
H= -6, K= 2		
1	243	237
2	408	-394
3	360	-342
4	207	-204
5	27	36
6	90	90
7	111	114
8	62	-59
9	102	-98
10	66	68
11	46	-42
H= -4, K= 2		
1	710	-709
2	229	-222
3	467	-464
4	122	127
5	163	-166
6	-17	-9
7	188	187
8	-20	2
9	108	99
10	95	95
11	-22	2
H= -2, K= 2		
1	216	209
2	78	68
3	93	-87
4	370	370
5	251	239
6	35	36
7	-18	-10
8	65	-68
9	-21	8
10	54	52
11	44	47
H= 1, K= 3		
0	150	-134
1	774	-775
2	640	-641
3	284	-278
4	130	-131
5	140	-138
6	182	187
7	-18	-26
8	-19	7
9	-20	1
10	-20	7
H= 3, K= 3		
0	678	675
1	463	-475
2	160	-169
3	112	114
4	133	-133

L	FO	FC
5	37	39
6	-18	-5
7	78	-80
8	-20	-4
9	-21	22
10	-21	1
H= 5, K= 3		
0	107	-102
1	130	131
2	25	25
3	327	326
4	135	145
5	122	114
6	47	40
7	-20	14
8	31	-36
9	-21	6
10	35	25
H= 7, K= 3		
0	279	-275
1	88	-93
2	54	-56
3	246	248
4	97	92
5	-18	-1
6	-19	5
7	-20	-2
8	-20	-16
9	-21	27
H= 9, K= 3		
0	117	-122
1	55	57
2	-17	26
3	39	38
4	-18	11
5	74	-73
6	57	-61
7	51	-52
8	45	-47
H= 11, K= 3		
0	193	-199
1	28	24
2	103	98
3	59	-57
4	32	37
5	107	-114
6	-20	15
7	-21	-3
8	-22	-2
H= 13, K= 3		
0	76	75
1	89	83
2	43	41
3	-20	-8
4	-21	-14
5	33	-27
6	-21	4
7	-22	20
H= 15, K= 3		
0	114	113
1	-20	9
2	74	77
3	-21	23
4	55	-53
5	-22	19
6	-22	-19

L	FO	FC
H= 17, K= 3		
0	-21	15
1	-21	-10
2	-21	3
3	46	-43
4	-22	-18
H= 19, K= 3		
0	-22	-9
1	37	41
2	53	-44
H= -21, K= 3		
1	53	-51
2	57	-59
3	-23	28
4	-22	1
H= -19, K= 3		
1	35	-25
2	81	-76
3	56	-62
4	-22	8
5	-23	-14
6	67	61
7	-23	-16
H= -17, K= 3		
1	42	41
2	-21	29
3	69	64
4	74	75
5	32	-38
6	36	40
7	-22	-17
8	-23	21
H= -15, K= 3		
1	45	58
2	-20	-7
3	43	50
4	121	125
5	36	39
6	-21	-3
7	-22	-10
8	38	-41
9	62	47
H= -13, K= 3		
1	46	41
2	-18	16
3	-19	9
4	52	-58
5	57	-57
6	110	-114
7	-21	-2
8	64	-64
9	-22	25
10	-22	-1
H= -11, K= 3		
1	31	-24
2	112	-111
3	86	-83
4	-18	1
5	89	-90
6	233	-237
7	53	-43
8	40	-32

L	FO	FC
9	-21	-17
10	-22	19
H= -9, K= 3		
1	43	33
2	77	-76
3	62	-68
4	136	131
5	-18	-1
6	96	95
7	141	144
8	98	101
9	-21	8
10	36	29
H= -7, K= 3		
1	235	236
2	175	180
3	41	-47
4	-16	1
5	94	96
6	102	105
7	84	91
8	221	225
9	77	78
10	-21	9
11	-22	3
H= -5, K= 3		
1	133	127
2	-15	-22
3	220	-212
4	153	-156
5	72	-61
6	92	-87
7	50	-49
8	-20	5
9	125	-121
10	75	-66
11	-22	18
H= -3, K= 3		
1	67	-84
2	557	559
3	94	93
4	157	-153
5	130	135
6	59	-66
7	-19	-26
8	84	-82
9	81	-78
10	119	-116
11	54	-48
H= -1, K= 3		
1	114	123
2	187	188
3	111	-113
4	58	72
5	242	235
6	66	65
7	26	-9
8	43	-35
9	-21	3
10	-21	-4
11	61	54
H= 0, K= 4		
0	343	-361
1	277	279
2	253	-241
3	73	-82

L	FO	FC
4	407	404
5	87	-94
6	35	36
7	95	91
8	-19	-20
9	-20	21
10	97	95

H= 2, K= 4

L	FO	FC
0	361	355
1	332	320
2	156	-146
3	121	-117
4	165	152
5	112	112
6	38	-30
7	79	79
8	-20	-5
9	-20	21
10	46	49

H= 4, K= 4

L	FO	FC
0	119	112
1	429	428
2	58	67
3	140	-140
4	76	76
5	34	-16
6	233	-240
7	31	-23
8	51	-48
9	38	-32

H= 6, K= 4

L	FO	FC
0	165	-170
1	79	-81
2	102	-103
3	81	-88
4	117	121
5	57	56
6	53	-43
7	124	-129
8	-21	20
9	48	-51

H= 8, K= 4

L	FO	FC
0	540	536
1	254	-253
2	-16	-5
3	122	-128
4	-18	10
5	134	141
6	58	-53
7	30	25
8	94	99

H= 10, K= 4

L	FO	FC
0	145	146
1	181	174
2	-18	2
3	-19	-1
4	-19	1
5	48	33
6	64	-69
7	-21	-3
8	36	30

H= 12, K= 4

L	FO	FC
0	27	-16
1	34	31
2	171	-173
3	54	55

L	FO	FC
4	-21	10
5	-20	15
6	-21	-8
7	62	-53

H= 14, K= 4

L	FO	FC
0	102	91
1	61	-61
2	111	-107
3	63	-61
4	-21	-7
5	-21	-2
6	-22	-10

H= 16, K= 4

L	FO	FC
0	-21	-3
1	-21	37
2	-21	-21
3	-21	-17
4	68	71

H= 18, K= 4

L	FO	FC
0	-21	11
1	-21	-4
2	40	-43
3	-23	20

H= 20, K= 4

L	FO	FC
0	-23	-11

H= -20, K= 4.

L	FO	FC
1	46	23
2	111	110
3	162	161
4	-23	0
5	42	36

H= -18, K= 4

L	FO	FC
1	33	-40
2	-22	18
3	-22	17
4	240	-240
5	-22	11
6	46	43
7	46	54

H= -16, K= 4

L	FO	FC
1	-21	22
2	33	39
3	68	-68
4	208	-209
5	256	-261
6	63	-58
7	35	-38
8	-23	12

H= -14, K= 4

L	FO	FC
1	32	37
2	-19	7
3	110	111
4	-20	-2
5	-21	-17
6	299	304
7	42	-49
8	52	-57
9	44	-47

H= -12, K= 4

L	FO	FC
1	36	27

L	FO	FC
2	-19	10
3	30	-40
4	132	-129
5	135	142
6	282	294
7	225	236
8	71	69
9	-21	-2
10	43	-30

H= -10, K= 4

L	FO	FC
1	266	-263
2	153	-164
3	75	-68
4	27	10
5	80	-84
6	-20	20
7	62	66
8	221	-219
9	-21	28
10	-22	20

H= -8, K= 4

L	FO	FC
1	37	-36
2	107	109
3	63	-66
4	-17	-26
5	62	59
6	165	171
7	65	-77
8	275	-276
9	117	-125
10	48	-49

H= -6, K= 4

L	FO	FC
1	421	412
2	173	-169
3	253	249
4	-16	10
5	82	-90
6	-18	-3
7	40	45
8	56	-59
9	-22	-28
10	141	134

H= -4, K= 4

L	FO	FC
1	202	-201
2	661	-665
3	275	277
4	36	29
5	31	-27
6	55	58
7	93	-92
8	125	-126
9	-21	25
10	169	171

H= -2, K= 4

L	FO	FC
1	112	-113
2	-15	38
3	254	-241
4	62	63
5	44	-42
6	-18	0
7	42	47
8	62	-59
9	88	-90
10	36	41

H= 1, K= 5

L	FO	FC
0	149	-138

L	FO	FC
1	112	-106
2	165	157
3	118	110
4	92	91
5	208	-206
6	212	-209
7	101	-94
8	-20	-4
9	66	60
10	-21	-1

H= 3, K= 5

L	FO	FC
0	50	58
1	79	-86
2	248	243
3	100	98
4	260	257
5	225	-226
6	65	68
7	-19	14
8	-20	16
9	-21	1

H= 5, K= 5

L	FO	FC
0	56	47
1	46	-63
2	-16	6
3	167	167
4	72	-74
5	89	-89
6	39	29
7	98	97
8	58	57
9	33	44

H= 7, K= 5

L	FO	FC
0	123	125
1	40	-38
2	46	-40
3	53	56
4	41	-42
5	56	-61
6	71	-64
7	97	98
8	-21	-21

H= 9, K= 5

L	FO	FC
0	53	44
1	233	-235
2	169	-165
3	-19	0
4	47	-47
5	71	-72
6	-21	15
7	60	62
8	-22	-11

H= 11, K= 5

L	FO	FC
0	160	165
1	157	-155
2	31	-27
3	-20	14
4	-20	-13
5	32	-36
6	31	-6
7	-21	26

H= 13, K= 5

L	FO	FC
0	-20	28
1	87	-86
2	79	78
3	87	91

L	FO	FC
4	114	115
5	-21	1
6	-21	0
H= 15, K= 5		
0	37	-44
1	-21	-5
2	114	-107
3	84	83
4	-22	19
5	-22	1
H= 17, K= 5		
0	-21	0
1	-22	-31
2	-21	-25
3	43	52
H= 19, K= 5		
0	-23	30
1	-22	-7
H= -19, K= 5		
1	37	-21
2	131	119
3	183	-179
4	-22	9
5	-23	28
H= -17, K= 5		
1	55	56
2	57	59
3	149	-145
4	101	105
5	89	92
6	72	68
7	-23	-9
H= -15, K= 5		
1	-21	11
2	-21	6
3	40	39
4	135	-135
5	263	263
6	-22	-16
7	-22	-18
8	38	-27
H= -13, K= 5		
1	51	-56
2	30	30
3	107	-111
4	89	-86
5	212	217
6	62	-64
7	87	-83
8	82	-80
9	-22	-14
H= -11, K= 5		
1	-18	7
2	-19	-25
3	45	-53
4	76	-81
5	-20	-11
6	187	191
7	253	-252
8	57	49
9	-22	-4

L	FO	FC
H= -9, K= 5		
1	81	-71
2	65	-66
3	67	66
4	93	-102
5	168	172
6	65	76
7	219	-227
8	86	90
9	66	71
10	90	85
H= -7, K= 5		
1	306	-296
2	179	-169
3	109	-107
4	41	-34
5	-19	32
6	-20	-3
7	-21	-37
8	223	-220
9	179	180
10	-22	0
H= -5, K= 5		
1	365	-354
2	31	22
3	122	119
4	245	242
5	34	-37
6	143	138
7	171	-169
8	75	-82
9	173	171
10	84	-83
H= -3, K= 5		
1	66	-59
2	220	-215
3	321	320
4	317	318
5	150	147
6	86	87
7	62	-68
8	-21	24
9	54	50
10	107	104
H= -1, K= 5		
1	196	-208
2	310	-299
3	345	327
4	261	-259
5	52	-47
6	132	-137
7	-20	33
8	78	-74
9	111	114
10	63	49
H= 0, K= 6		
0	263	260
1	153	-151
2	197	196
3	110	-105
4	54	-45
5	60	62
6	-19	17
7	42	-36
8	35	28
9	-21	-2

L	FO	FC
H= 2, K= 6		
0	206	195
1	136	144
2	73	-68
3	152	148
4	26	-10
5	32	29
6	-19	32
7	33	-34
8	39	-29
9	-21	-15
H= 4, K= 6		
0	197	-191
1	217	-221
2	190	-192
3	82	76
4	122	-115
5	115	111
6	-19	-4
7	-20	8
8	54	-42
9	-22	30
H= 6, K= 6		
0	165	-151
1	62	-56
2	138	-139
3	104	-102
4	47	46
5	85	-82
6	52	45
7	-20	7
8	-21	0
H= 8, K= 6		
0	31	24
1	237	231
2	93	93
3	32	31
4	94	94
5	86	-87
6	81	78
7	68	-64
H= 10, K= 6		
0	70	-59
1	-19	16
2	54	61
3	91	84
4	-20	23
5	61	62
6	-21	-25
7	-22	26
H= 12, K= 6		
0	50	-42
1	-20	5
2	-21	22
3	66	-72
4	-21	-34
5	-21	-2
6	41	-28
H= 14, K= 6		
0	-21	-18
1	42	25
2	54	50
3	37	-35
4	-22	-24
5	34	-35

L	FO	FC
H= 16, K= 6		
0	-21	8
1	44	-49
2	-22	12
3	-22	-9
H= 18, K= 6		
0	39	-43
1	34	-40
H= -18, K= 6		
1	73	76
2	111	-110
3	83	81
4	-22	0
5	47	-32
H= -16, K= 6		
1	44	-46
2	-21	-3
3	58	58
4	45	27
5	70	73
6	47	-49
7	80	-78
H= -14, K= 6		
1	85	-89
2	56	55
3	146	-150
4	179	176
5	75	-85
6	-21	22
7	59	51
8	-22	12
H= -12, K= 6		
1	118	-116
2	55	-47
3	-20	18
4	34	-14
5	154	-147
6	-21	-27
7	45	-44
8	61	55
9	99	95
H= -10, K= 6		
1	138	133
2	-19	42
3	130	132
4	48	-60
5	176	174
6	196	-205
7	57	59
8	-21	6
9	-22	-8
H= -8, K= 6		
1	50	58
2	95	86
3	152	159
4	35	27
5	-20	-18
6	44	-35
7	106	108
8	-21	7
9	-22	-11

L	FO	FC
H= -6, K= 6		
1	129	-136
2	119	117
3	104	-100
4	40	-43
5	33	-27
6	39	50
7	118	-120
8	144	143
9	73	-76
H= -4, K= 6		
1	309	320
2	-16	-31
3	146	-149
4	-18	-8
5	42	-36
6	-19	5
7	34	29
8	46	48
9	71	-67
10	-22	-18
H= -2, K= 6		
1	94	-96
2	71	51
3	-16	-7
4	135	-133
5	-18	-21
6	63	58
7	-21	3
8	-21	-30
9	105	101
H= 1, K= 7		
0	24	0
1	30	13
2	39	-37
3	53	51
4	43	38
5	42	-35
6	83	80
7	35	23
8	-21	1
9	-21	24
H= 3, K= 7		
0	-17	-28
1	65	-81
2	37	-48
3	52	-52
4	93	92
5	-19	-17
6	37	28
7	46	41
8	-21	16
H= 5, K= 7		
0	186	196
1	71	-66
2	-18	17
3	-19	-6
4	-19	0
5	-20	-4
6	-21	-37
7	55	43
8	-22	-21
H= 7, K= 7		
0	41	24

L	FO	FC
1	63	58
2	79	77
3	45	45
4	-21	6
5	-20	14
6	61	-58
7	-22	7
H= 9, K= 7		
0	-19	-36
1	-19	6
2	72	-71
3	-20	9
4	-20	-4
5	33	-25
6	-21	-7
H= 11, K= 7		
0	50	-51
1	97	-91
2	57	-55
3	-20	16
4	60	-56
5	40	-29
H= 13, K= 7		
0	-20	0
1	72	-71
2	-21	-10
3	-21	-14
4	32	20
H= 15, K= 7		
0	-21	12
1	-22	-9
2	-21	24
3	-22	19
H= 17, K= 7		
0	-22	17
H= -17, K= 7		
1	53	-44
2	-23	37
3	-23	-34
4	-23	-22
H= -15, K= 7		
1	48	51
2	57	-61
3	50	-51
4	-21	-5
5	63	53
6	77	66
H= -13, K= 7		
1	-21	54
2	58	-56
3	-21	25
4	100	-94
5	-21	29
6	-21	2
7	40	-48
H= -11, K= 7		
1	-20	-3
2	38	33
3	49	-59
4	101	108

L	FO	FC
5	55	64
6	-21	-20
7	83	-83
8	67	-68
H= -9, K= 7		
1	49	-64
2	-19	21
3	36	-54
4	111	124
5	-21	-25
6	113	109
7	91	-86
8	33	-23
H= -7, K= 7		
1	227	-225
2	42	39
3	59	58
4	54	-40
5	73	82
6	63	-64
7	52	-52
8	-21	24
9	45	40
H= -5, K= 7		
1	65	-63
2	40	57
3	82	82
4	48	-58
5	102	107
6	110	-112
7	61	66
8	65	-60
9	84	78
H= -3, K= 7		
1	80	85
2	-17	4
3	101	95
4	90	-100
5	100	-100
6	-19	-6
7	51	-60
8	-21	31
9	49	45
H= -1, K= 7		
1	-17	-12
2	145	-148
3	87	85
4	-18	-8
5	118	-113
6	-20	14
7	67	-68
8	41	55
9	44	-39
H= 0, K= 8		
0	40	48
1	-18	20
2	60	-62
3	47	41
4	43	-44
5	53	50
6	29	-11
7	-21	25
8	54	-48
H= 2, K= 8		

L	FO	FC
0	35	28
1	355	369
2	56	-62
3	-19	18
4	81	-89
5	-20	-1
6	-20	0
7	41	36
8	-21	-3
H= 4, K= 8		
0	125	129
1	52	62
2	53	-50
3	-20	-16
4	-20	-7
5	45	-34
6	46	52
7	-21	-19
H= 6, K= 8		
0	39	31
1	48	-51
2	70	-72
3	211	-220
4	-21	-12
5	-20	-8
6	-21	29
7	-22	-7
H= 8, K= 8		
0	67	-69
1	-20	-27
2	59	-73
3	71	-69
4	45	42
5	30	4
6	-22	4
H= 10, K= 8		
0	-21	28
1	-21	-29
2	-21	-6
3	-21	12
4	97	95
5	134	134
H= 12, K= 8		
0	-20	11
1	38	41
2	-21	-16
3	-21	0
4	38	50
H= 14, K= 8		
0	-21	-19
1	-21	-17
2	-22	-22
H= 16, K= 8		
0	34	-33
H= -16, K= 8		
1	55	-50
2	-22	13
3	40	-19
H= -14, K= 8		
1	-22	-38

L	FO	FC
2	-22	30
3	-22	-23
4	62	-51
5	-23	-31
6	52	-51
H= -12, K= 8		
1	-20	2
2	82	91
3	81	88
4	-21	2
5	40	34
6	94	-83
7	-22	16
H= -10, K= 8		
1	38	-44
2	53	55
3	-21	50
4	-21	3
5	66	66
6	55	60
7	-22	23
H= -8, K= 8		
1	49	43
2	81	-82
3	32	-32
4	92	-100
5	93	-86
6	-21	17
7	-22	-20
8	75	69
H= -6, K= 8		
1	28	-26
2	81	-82
3	79	74
4	60	-64
5	51	-71
6	-20	0
7	46	-46
8	-22	-5
H= -4, K= 8		
1	-18	-22
2	120	121
3	45	-45
4	29	22
5	-20	6
6	42	48
7	-21	30
8	-21	2
H= -2, K= 8		
1	77	-69
2	82	75
3	-19	16
4	72	83
5	58	-59
6	-20	15
7	41	59
8	-21	-1
H= 1, K= 9		
0	106	104
1	402	-422
2	144	-143
3	33	-34
4	32	34
5	30	28

L	FO	FC
6	-20	13
7	-21	-26
H= 3, K= 9		
0	132	136
1	362	-371
2	93	-87
3	45	-40
4	-20	-9
5	69	-71
6	29	6
H= 5, K= 9		
0	40	30
1	43	23
2	73	-68
3	317	320
4	110	108
5	-21	26
6	36	-18
H= 7, K= 9		
0	78	78
1	58	-60
2	145	-144
3	296	287
4	60	53
5	60	60
H= 9, K= 9		
0	-21	16
1	109	-98
2	-21	-6
3	-21	-15
4	46	38
H= 11, K= 9		
0	-21	-14
1	51	45
2	48	-50
3	33	33
H= 13, K= 9		
0	-22	-13
1	40	36
H= -13, K= 9		
1	-22	34
2	-22	27
3	-22	-7
4	-22	-7
5	-22	13
H= -11, K= 9		
1	51	-38
2	55	56
3	113	-124
4	33	-45
5	-21	-16
6	-22	30
H= -9, K= 9		
1	42	39
2	-20	20
3	92	-96
4	55	-54
5	-21	2
6	-22	16

L	FO	FC
H= -7, K= 9		
1	90	96
2	-20	17
3	-20	-8
4	44	-55
5	82	101
6	-21	42
7	-22	35
H= -5, K= 9		
1	52	-56
2	-20	1
3	31	-48
4	-21	-36
5	77	77
6	34	32
7	-22	-26
H= -3, K= 9		
1	47	-46
2	67	-69
3	56	-52
4	-20	-23
5	53	52
6	49	50
7	92	-100
H= -1, K= 9		
1	-20	-4
2	-19	-13
3	48	54
4	-20	12
5	86	95
6	-21	41
7	40	-46
H= 0, K= 10		
0	32	41
1	28	10
2	85	85
3	58	48
4	-20	-1
5	-21	3
6	38	22
H= 2, K= 10		
0	147	-143
1	-20	-20
2	146	142
3	135	133
4	32	44
5	64	63
H= 4, K= 10		
0	122	-136
1	-20	8
2	-20	4
3	-20	-8
4	-21	-23
5	33	-19
H= 6, K= 10		
0	-20	24
1	122	-120
2	115	115
3	-22	6
4	73	-74
H= 8, K= 10		

L	FO	FC
0	-21	-7
1	95	-92
2	98	97
3	-22	14
H= 10, K= 10		
0	-22	-35
1	-21	5
2	-22	-6
H= 12, K= 10		
0	-22	-21
H= -12, K= 10		
1	-22	22
2	67	-62
H= -10, K= 10		
1	-21	26
2	75	-83
3	-21	-6
4	-22	-8
H= -8, K= 10		
1	31	-22
2	58	63
3	41	-28
4	48	59
5	-22	-14
H= -6, K= 10		
1	62	58
2	58	67
3	32	-29
4	112	111
5	-21	0
6	-22	-9
H= -4, K= 10		
1	103	-104
2	-20	-9
3	-20	16
4	45	-50
5	-21	23
6	-22	-31
H= -2, K= 10		
1	160	-157
2	71	-65
3	77	-72
4	40	-56
5	31	41
6	67	-64
H= 1, K= 11		
0	31	9
1	-20	15
2	36	-14
3	-21	-16
4	56	-54
H= 3, K= 11		
0	-21	26
1	32	-8
2	-21	14
3	-21	4

L	FO	FC
H=	5, K=	11
0	-21	-27
1	-21	-32
2	-21	-13
3	38	-35
H=	7, K=	11
0	79	-72
1	54	40

L	FO	FC
2	45	-38
H=	-9, K=	11
1	37	-29
H=	-7, K=	11
1	63	-52
2	51	-52
3	-22	-10

L	FO	FC
H=	-5, K=	11
1	-21	-22
2	65	-67
3	-21	30
4	-21	4
H=	-3, K=	11
1	-21	31
2	58	61
3	35	35

L	FO	FC
4	47	56
H=	-1, K=	11
1	-20	2
2	-21	17
3	-21	11
4	61	54
H=	0, K=	12
0	107	-106

Table B-4

Observed and Calculated Structure Factors for $[Ni_2C\ell(H_2O)_4$-(dhphpy)$]C\ell_3 \cdot 2H_2O$

L	FO	FC
H=	0, K=	0
2	563	-490
4	1938	-2036
6	563	598
8	135	-253
10	659	-607
12	314	-323
14	-64	103
16	130	-183
18	148	113
20	242	261
22	177	184
24	115	-142
26	700	-691
H=	2, K=	0
0	483	373
2	2936	-2814
4	137	-124
6	345	-303
8	1693	1682
10	124	-119
12	115	107
14	645	649
16	555	-547
18	255	251
20	348	362
22	342	-354
24	413	-402
26	311	292
-28	549	-541
-26	448	-459
-24	206	181
-22	426	443
-20	111	-109
-18	269	-274
-16	860	846
-14	568	-551
-12	283	-322
-10	273	332
-8	2573	-2519
-6	1888	-1666
-4	329	-390
-2	3358	3505
H=	4, K=	0
0	7329	-8496
2	242	-231
4	1140	1162
6	305	-285
8	351	-306
10	99	120
12	425	433
14	199	-227
16	-80	86
18	-80	27
20	271	-285
22	195	-158
-30	469	-434
-28	396	-389
-26	574	573
-24	218	209
-22	216	-217
-20	427	-417
-18	192	162
-16	674	657
-14	134	126
-12	310	246
-10	565	542
-8	659	588
-6	219	-147
-4	427	380
-2	1524	1519

L	FO	FC
H=	6, K=	0
0	1163	-1171
2	3015	2987
4	911	905
6	363	-391
8	965	-1004
10	317	322
12	-79	6
14	445	-434
16	225	230
18	138	-93
20	-84	-106
-30	602	-576
-28	550	567
-26	747	754
-24	349	-388
-22	765	-780
-20	163	185
-18	296	315
-16	929	-921
-14	167	197
-12	157	119
-10	147	-99
-8	1553	1483
-6	973	936
-4	816	741
-2	2496	-2505
H=	8, K=	0
0	3957	4100
2	411	421
4	429	-436
6	252	278
8	-76	-83
10	-81	-128
12	196	-195
14	-79	57
16	-81	-11
-30	472	474
-28	521	526
-26	341	-332
-24	-78	18
-22	-78	-24
-20	-77	92
-18	139	168
-16	448	-446
-14	315	-276
-12	126	109
-10	277	-252
-8	138	100
-6	-65	46
-4	1229	-1237
-2	1643	-1668
H=	10, K=	0
0	655	660
2	942	-965
4	424	-438
6	-80	95
8	529	527
10	257	-265
12	140	-153
-30	514	502
-28	226	-223
-26	539	-552
-24	113	129
-22	668	675
-20	131	-135
-18	642	-619
-16	759	758
-14	343	349
-12	-72	57
-10	319	325
-8	574	-580
-6	519	-544

L	FO	FC
-4	412	-419
-2	607	632
H=	12, K=	0
0	1691	-1722
2	494	-506
4	427	434
6	-87	152
8	-84	-75
-28	551	-541
-26	211	200
-24	194	187
-22	142	-126
-20	382	-399
-18	127	-177
-16	347	357
-14	249	256
-12	181	-180
-10	-79	38
-8	-79	61
-6	-80	-14
-4	374	362
-2	1073	1111
H=	14, K=	0
0	586	-594
2	433	436
-24	-83	-16
-22	346	-328
-20	-81	66
-18	284	277
-16	306	-328
-14	171	-187
-12	-81	-111
-10	197	-226
-8	141	136
-6	394	399
-4	371	360
-2	378	-411
H=	16, K=	0
-16	322	-311
-14	205	-207
-12	192	202
-10	-84	5
H=	1, K=	1
0	1935	2098
1	1346	-1410
2	1854	-1916
3	617	-569
4	1209	-1108
5	712	-736
6	347	323
7	338	-273
8	187	-142
9	172	193
10	256	-241
11	700	-693
12	1185	1242
13	-70	46
14	438	437
15	793	797
16	-76	145
17	310	335
18	358	-364
19	-82	-57
20	551	565
21	251	-253
22	-82	-47
23	336	-356
24	670	-656
25	-91	184
26	-85	-23

L	FO	FC
-28	194	-212
-27	-93	-106
-26	284	-325
-25	217	253
-24	-93	-193
-23	290	382
-22	363	384
-21	-96	-60
-20	227	-375
-19	326	-352
-18	-92	-25
-17	-98	-422
-16	-90	412
-15	-96	-68
-14	-96	-292
-13	553	595
-12	-98	188
-11	498	-522
-10	190	-247
-9	847	-807
-8	445	512
-7	201	-232
-6	798	-785
-5	1418	1462
-4	827	-696
-3	393	244
-2	857	728
-1	124	51
H=	3, K=	1
0	758	-639
1	348	317
2	-70	-126
3	381	-331
4	390	-408
5	559	559
6	-67	19
7	-67	-43
8	472	-485
9	447	-461
10	-66	-92
11	500	-516
12	-69	59
13	621	605
14	199	238
15	301	299
16	475	-478
17	386	-382
18	-81	51
19	426	-455
20	411	398
21	-82	-59
22	450	-430
23	273	243
24	-84	44
-29	-103	-181
-28	-100	-238
-27	264	291
-26	138	-171
-25	200	249
-24	569	577
-23	406	-433
-22	316	327
-21	233	-240
-20	683	-670
-19	-74	-104
-18	571	573
-17	392	392
-16	352	362
-15	1384	1345
-14	643	-681
-13	105	-108
-12	1674	-1524
-11	1773	-1789
-10	723	630
-9	-67	88
-8	148	-143

L	FO	FC
-7	281	230
-6	753	-765
-5	697	-574
-4	1044	1036
-3	459	-483
-2	1737	1655
-1	1005	-945
H= 5, K= 1		
0	1566	-1596
1	942	945
2	958	923
3	465	439
4	1415	1442
5	350	372
6	340	-347
7	390	-379
8	335	-338
9	356	-360
10	570	553
11	645	640
12	452	-450
13	176	218
14	365	-342
15	466	-452
16	230	-205
17	204	-229
18	-81	124
19	-81	-11
20	276	-276
21	-84	79
22	-84	3
-30	561	-545
-29	245	240
-28	-81	-14
-27	-82	152
-26	421	415
-25	219	-236
-24	319	293
-23	582	-568
-22	687	-681
-21	-77	4
-20	383	369
-19	551	583
-18	519	488
-17	690	694
-16	506	-477
-15	123	55
-14	-64	55
-13	702	-622
-12	566	-560
-11	328	285
-10	443	393
-9	140	148
-8	425	408
-7	319	275
-6	345	297
-5	476	-449
-4	109	110
-3	-68	-70
-2	505	448
-1	-68	93
H= 7, K= 1		
0	473	456
1	-67	-62
2	812	843
3	-68	65
4	-69	-6
5	428	-443
6	-72	-86
7	-73	-55
8	360	379
9	-77	105
10	-78	67
11	219	222

L	FO	FC
12	117	38
13	123	-155
14	175	-151
15	-80	-67
16	149	153
17	-84	150
18	126	70
19	251	254
-30	-84	33
-29	200	223
-28	486	473
-27	312	-317
-26	295	266
-25	338	-339
-24	477	-484
-23	393	407
-22	314	-331
-21	246	208
-20	481	477
-19	-73	22
-18	450	-455
-17	-70	-15
-16	337	-328
-15	832	-829
-14	212	209
-13	292	-278
-12	1029	1043
-11	1070	1055
-10	395	-403
-9	-70	70
-8	-70	17
-7	485	-480
-6	997	963
-5	-70	-36
-4	886	-880
-3	574	587
-2	2150	-2151
-1	1041	1025
H= 9, K= 1		
0	700	712
1	348	-347
2	187	-153
3	-77	-53
4	443	-447
5	213	-246
6	-80	-27
7	-80	43
8	119	83
9	129	150
10	272	-286
11	243	-258
12	-81	41
13	221	-199
14	162	146
15	256	232
-30	497	491
-29	196	-210
-28	164	177
-27	161	-140
-26	156	-129
-25	-80	39
-24	311	-305
-23	441	428
-22	355	349
-21	-78	11
-20	127	-109
-19	373	-349
-18	474	-480
-17	545	-555
-16	264	286
-15	-72	-5
-14	352	321
-13	900	887
-12	415	427
-11	-59	-97
-10	270	-265

L	FO	FC
-9	735	-721
-8	144	157
-7	517	-504
-6	206	-191
-5	428	431
-4	385	-385
-3	203	210
-2	448	-455
-1	-73	-39
H= 11, K= 1		
0	-82	34
1	-82	58
2	391	-378
3	-80	-44
4	-81	-4
5	271	270
6	221	226
7	-82	77
8	234	-199
9	171	-137
10	236	-214
11	228	-237
-29	242	-240
-28	329	-307
-27	205	215
-26	357	-349
-25	307	300
-24	300	306
-23	297	-295
-22	298	283
-21	316	-302
-20	632	-630
-19	155	-148
-18	117	120
-17	-80	89
-16	524	541
-15	753	770
-14	-78	13
-13	249	275
-12	579	-554
-11	594	-601
-10	143	151
-9	-77	-105
-8	-76	-23
-7	128	87
-6	297	-287
-5	-78	-39
-4	290	292
-3	141	-144
-2	895	904
-1	407	-427
H= 13, K= 1		
0	611	-641
1	228	254
2	-83	-16
3	-84	71
4	379	364
5	149	141
-27	124	108
-26	187	175
-25	-84	-35
-24	256	259
-23	320	-340
-22	303	-298
-21	-79	-47
-20	-79	-6
-19	213	179
-18	303	318
-17	227	248
-16	156	-112
-15	116	110
-14	140	-124
-13	308	-326
-12	359	-356

L	FO	FC
-11	-81	-21
-10	-80	32
-9	201	245
-8	-82	-108
-7	299	332
-6	-80	-10
-5	257	-240
-4	319	322
-3	225	-218
-2	357	369
-1	-84	17
H= 15, K= 1		
-22	158	-118
-21	126	162
-20	277	273
-19	-85	58
-18	-84	55
-17	-84	9
-16	297	-277
-15	415	-415
-14	-85	-113
-13	208	-219
-12	300	302
-11	416	414
-10	-85	-85
-9	188	174
-8	-85	-31
-7	181	-173
-6	252	258
-5	157	-123
-4	-86	-14
-3	-87	47
H= 0, K= 2		
0	321	-349
1	90	250
2	761	-703
3	238	-327
4	402	425
5	614	-490
6	143	67
7	875	821
8	550	537
9	650	662
10	376	-376
11	-71	-8
12	715	-742
13	1073	-1096
14	975	981
15	-73	-38
16	409	426
17	-86	-31
18	432	-457
19	-94	-60
20	264	-311
21	235	-230
22	-35	86
23	240	-274
24	276	-359
25	323	312
26	267	-255
27	-88	65
H= 2, K= 2		
0	94	58
1	183	-122
2	195	129
3	94	12
4	499	510
5	547	589
6	1059	-1048
7	300	318
8	-67	-23
9	875	860

L	FO	FC
10	366	-339
11	756	-760
12	1086	1099
13	-71	-62
14	380	401
15	1101	1109
16	410	-423
17	146	-163
18	263	-318
19	749	-756
20	-84	-28
21	-80	-48
22	173	158
23	-81	-31
24	159	-154
25	-86	35
-29	-89	-37
-28	158	-147
-27	-94	32
-26	305	-321
-25	-84	-3
-24	-81	28
-23	-82	-142
-22	-81	-59
-21	-82	31
-20	-115	200
-19	717	-717
-18	-82	143
-17	499	-541
-16	655	660
-15	1196	1184
-14	-66	-120
-13	-72	111
-12	2017	-1984
-11	1867	-1741
-10	408	369
-9	431	332
-8	797	786
-7	1049	1154
-6	754	708
-5	1507	1321
-4	1370	-1344
-3	120	1
-2	352	-380
-1	152	-211

H= 4, K= 2

L	FO	FC
0	534	534
1	526	-547
2	266	299
3	129	-163
4	401	-395
5	438	414
6	290	-286
7	665	-673
8	555	-544
9	983	-965
10	636	641
11	113	-107
12	1036	1023
13	1170	1164
14	868	-887
15	-80	100
16	585	-564
17	168	-224
18	234	227
19	-81	22
20	164	152
21	197	168
22	-85	-105
23	231	217
-30	-86	44
-29	-87	140
-28	343	-318
-27	-82	90
-26	-81	92
-25	465	465
-24	541	520
-23	143	-195
-22	-79	-52
-21	259	-269
-20	429	428
-19	-75	-71
-18	1108	1065
-17	382	375
-16	473	-477
-15	228	223
-14	[illegible]	-1630
-13	1572	-1679
-12	737	721
-11	397	-375
-10	614	619
-9	804	754
-8	293	-263
-7	550	602
-6	886	893
-5	-69	-32
-4	418	-397
-3	-70	-82
-2	371	364
-1	-69	-164

H= 6, K= 2

L	FO	FC
0	542	-523
1	352	355
2	238	245
3	374	390
4	495	-482
5	360	-365
6	253	259
7	401	-435
8	357	349
9	507	-501
10	591	598
11	372	402
12	461	-460
13	121	68
14	253	-251
15	573	-542
16	-82	38
17	-80	17
18	143	92
19	365	340
20	127	101
-30	404	-408
-29	-85	78
-28	-80	12
-27	-82	-82
-26	420	438
-25	-81	18
-24	-80	-30
-23	-79	74
-22	131	57
-21	-78	-70
-20	-75	-14
-19	662	653
-18	128	-124
-17	633	606
-16	746	-737
-15	685	-666
-14	561	-546
-13	-66	3
-12	1039	967
-11	986	952
-10	115	84
-9	315	-331
-8	-68	-58
-7	341	-327
-6	422	-444
-5	708	-739
-4	1155	1183
-3	107	-106
-2	226	247
-1	377	366

H= 8, K= 2

L	FO	FC
0	337	-342
1	131	256
2	214	-243
3	242	242
4	152	163
5	145	-140
6	113	116
7	260	282
8	150	118
9	260	275
10	161	-142
11	170	155
12	497	-496
13	455	-477
14	288	298
15	-84	-95
16	335	343
17	170	179
-30	127	-126
-29	153	-156
-28	333	322
-27	-79	-50
-26	-79	128
-25	472	-476
-24	387	-410
-23	127	98
-22	-79	-66
-21	-78	6
-20	261	-229
-19	-76	-14
-18	738	-732
-17	-73	-27
-16	-71	76
-15	362	-348
-14	1058	1074
-13	1053	1027
-12	230	-222
-11	637	661
-10	853	-843
-9	831	-853
-8	132	140
-7	1146	-1108
-6	144	105
-5	194	189
-4	137	157
-3	437	436
-2	572	-549
-1	121	136

H= 10, K= 2

L	FO	FC
0	343	319
1	186	-189
2	-79	-52
3	232	-243
4	213	212
5	-79	74
6	116	-120
7	135	174
8	180	-181
9	246	259
10	483	-501
11	291	-305
12	166	179
13	152	-137
-30	303	291
-29	151	-118
-28	121	120
-27	-80	71
-26	302	-340
-25	-78	-19
-24	-79	-89
-23	-80	-42
-22	-80	-3
-21	133	142
-20	118	-136
-19	470	-463
-18	-76	14
-17	545	-563
-16	934	952
-15	744	763
-14	576	587
-13	465	456
-12	1029	-1004
-11	924	-918
-10	151	-135
-9	179	-192
-8	284	255
-7	178	166
-6	206	214
-5	290	279
-4	433	-432
-3	-75	137
-2	-76	-131
-1	-77	-94

H= 12, K= 2

L	FO	FC
0	281	237
1	-81	-60
2	-82	67
3	140	-142
4	-82	23
5	155	174
6	131	-71
7	-85	-91
8	186	-184
-28	247	-260
-27	-86	5
-26	258	-270
-25	355	351
-24	336	315
-23	131	-71
-22	-79	-37
-21	-80	-52
-20	-81	41
-19	-81	24
-18	603	604
-17	-83	52
-16	119	97
-15	285	287
-14	520	-515
-13	390	-390
-12	-81	-84
-11	284	-284
-10	122	115
-9	245	227
-8	-80	-77
-7	457	466
-6	-80	66
-5	-80	46
-4	142	-108
-3	171	-146
-2	378	372
-1	-83	-114

H= 14, K= 2

L	FO	FC
0	241	-236
1	151	65
2	-86	24
-25	-85	5
-24	-84	93
-23	-83	42
-22	-82	19
-21	121	-103
-20	-81	92
-19	-83	108
-18	-83	64
-17	252	265
-16	341	-359
-15	281	-281
-14	417	-412

L	FO	FC
-13	303	-317
-12	402	415
-11	406	410
-10	132	121
-9	273	272
-8	325	-320
-7	-81	-66
-6	150	-171
-5	303	-304
-4	378	347
-3	-85	-96
-2	170	120
-1	141	106

H= 16, K= 2

L	FO	FC
-16	143	-150
-15	271	-282
-14	307	358
-13	220	241
-12	197	199
-11	349	324

H= 1, K= 3

L	FO	FC
0	243	-269
1	989	947
2	620	684
3	-69	25
4	940	853
5	677	-686
6	513	565
7	-67	-7
8	918	-902
9	557	521
10	331	-364
11	123	-189
12	495	527
13	356	-507
14	-91	351
15	-95	249
16	547	590
17	-115	87
18	906	-986
19	-116	-593
20	-100	-238
21	415	460
22	-94	220
23	210	274
24	-90	-187
25	-87	109
26	206	211
-28	140	148
-27	127	139
-26	-82	81
-25	-87	-200
-24	491	-488
-23	-83	-73
-22	172	204
-21	651	651
-20	325	-355
-19	-78	143
-18	402	415
-17	214	-223
-16	657	662
-15	174	160
-14	271	296
-13	-71	-86
-12	1523	-1529
-11	617	-621
-10	1873	-1803
-9	416	-402
-8	1357	1283
-7	1544	1493
-6	598	-503
-5	1175	1208
-4	339	-356
-3	126	-119
-2	1489	1483
-1	-64	181

H= 3, K= 3

L	FO	FC
0	-68	-30
1	-68	8
2	1777	-1730
3	335	418
4	284	-292
5	685	674
6	597	583
7	954	964
8	1112	-1116
9	-66	-55
10	955	928
11	588	-598
12	1624	1634
13	-77	-5
14	-76	-34
15	256	253
16	831	-851
17	335	-339
18	494	-473
19	-82	-39
20	395	401
21	636	621
22	189	-204
23	-86	24
24	317	289
-29	-35	142
-28	-86	-85
-27	-98	-119
-26	269	-308
-25	-91	170
-24	-88	227
-23	253	239
-22	-87	-176
-21	727	742
-20	-31	148
-19	655	-674
-18	1485	1508
-17	-74	-119
-16	312	-307
-15	540	510
-14	937	-928
-13	903	-826
-12	1017	-1008
-11	859	-871
-10	1038	1072
-9	802	808
-8	1656	1549
-7	478	391
-6	863	-808
-5	1071	-1007
-4	566	-606
-3	356	-385
-2	608	-536
-1	-69	119

H= 5, K= 3

L	FO	FC
0	365	351
1	758	-770
2	378	-429
3	137	-122
4	737	-793
5	892	944
6	779	-754
7	113	131
8	710	693
9	723	-717
10	915	899
11	-77	65
12	258	-240
13	376	330
14	368	-390
15	298	-289
16	483	-471
17	136	-157
18	436	418
19	350	359
20	154	141
21	250	-235
-30	-84	69
-29	139	-100
-28	278	-297
-27	209	-233
-26	232	-226
-25	319	333
-24	560	550
-23	279	272
-22	177	-161
-21	810	-799
-20	596	572
-19	345	-349
-18	263	-247
-17	345	352
-16	943	-946
-15	139	-160
-14	602	-558
-13	165	183
-12	913	900
-11	747	696
-10	1502	1509
-9	491	523
-8	115	-154
-7	492	-478
-6	1037	1060
-5	644	-597
-4	342	315
-3	363	-375
-2	874	-879
-1	295	-286

H= 7, K= 3

L	FO	FC
0	262	-287
1	214	-182
2	634	646
3	236	238
4	-70	57
5	-73	-113
6	207	-203
7	397	-403
8	684	711
9	-79	-57
10	287	-295
11	221	197
12	760	-772
13	-83	68
14	-80	-36
15	130	-87
16	281	277
17	133	110
18	361	333
-30	285	-277
-29	269	-262
-28	-81	45
-27	163	183
-26	308	337
-25	-80	-97
-24	144	-100
-23	221	-197
-22	240	226
-21	815	-840
-20	-77	-76
-19	201	211
-18	1237	-1192
-17	-74	107
-16	162	133
-15	237	-240
-14	-68	105
-13	515	485
-12	531	558
-11	716	680
-10	436	-410
-9	316	-282
-8	1335	-1311
-7	528	-519
-6	528	537
-5	780	757
-4	807	811
-3	531	515
-2	222	219
-1	583	-621

H= 9, K= 3

L	FO	FC
0	245	-239
1	203	191
2	204	201
3	-78	78
4	275	297
5	278	-276
6	212	219
7	125	-133
8	225	-230
9	280	310
10	441	-453
11	-81	60
12	-83	-27
13	233	-220
14	233	257
15	196	166
-30	133	-117
-29	-83	54
-28	295	293
-27	249	250
-26	332	336
-25	183	-162
-24	444	-461
-23	208	-193
-22	156	165
-21	468	478
-20	277	-289
-19	370	393
-18	-77	-47
-17	273	-275
-16	737	735
-15	-75	1
-14	910	903
-13	161	158
-12	775	-783
-11	481	-481
-10	1555	-1529
-9	827	-817
-8	439	435
-7	303	303
-6	-71	-74
-5	495	503
-4	337	-339
-3	-73	31
-2	266	275
-1	-73	40

H= 11, K= 3

L	FO	FC
0	205	206
1	-81	49
2	197	-215
3	206	-214
4	-79	19
5	-60	-57
6	-81	81
7	239	258
8	510	-507
9	-85	106
10	-85	-8
-29	196	188
-28	-80	30
-27	141	-141
-26	261	-274
-25	-80	29

L	FO	FC
-24	-79	-8
-23	-80	133
-22	292	-293
-21	766	781
-20	153	-80
-19	-82	-106
-18	1002	1005
-17	202	-197
-16	117	150
-15	299	301
-14	171	-193
-13	224	-226
-12	350	-359
-11	445	-449
-10	-78	90
-9	-78	96
-8	515	502
-7	299	289
-6	-79	-80
-5	150	-152
-4	190	-172
-3	126	-111
-2	-81	-113
-1	216	203

H= 13, K= 3

L	FO	FC
0	181	188
1	198	-160
2	-83	-73
3	187	-172
4	152	-153
5	154	168
-26	357	-353
-25	-85	83
-24	286	263
-23	197	214
-22	-82	-100
-21	220	-213
-20	175	153
-19	290	-294
-18	143	116
-17	-80	44
-16	226	-223
-15	-80	-60
-14	478	-494
-13	-80	-68
-12	118	118
-11	202	186
-10	629	645
-9	367	381
-8	173	-178
-7	-81	-7
-6	133	-130
-5	203	-230
-4	134	162
-3	-81	71
-2	-81	63
-1	131	114

H= 15, K= 3

L	FO	FC
-21	377	-386
-20	-88	118
-19	-86	-42
-18	454	-433
-17	151	127
-16	-86	-131
-15	188	-190
-14	-86	69
-13	-83	9
-12	329	322
-11	290	282
-10	-85	-60
-9	-83	9
-8	457	-445
-7	261	-288
-6	-86	14
-5	-85	31
-4	184	192

H= 0, K= 4

L	FO	FC
0	350	316
1	1399	1346
2	516	-539
3	1039	981
4	279	333
5	597	-581
6	-57	-82
7	1431	-1418
8	-69	-24
9	466	435
10	153	-120
11	315	322
12	226	-221
13	-66	10
14	1093	1098
15	466	484
16	343	365
17	249	-282
18	151	-207
19	1006	-1005
20	260	-269
21	143	120
22	-81	112
23	297	303
24	-85	44
25	160	202
26	-96	-145
27	411	-459

H= 2, K= 4

L	FO	FC
0	238	324
1	795	768
2	563	-626
3	474	-463
4	116	-51
5	434	428
6	1033	-1082
7	423	431
8	532	-569
9	815	802
10	124	-142
11	210	216
12	877	858
13	230	230
14	288	296
15	257	-245
16	-81	-88
17	713	-713
18	-85	-101
19	-80	-19
20	-84	99
21	554	556
22	-87	6
23	213	180
24	-84	-7
25	302	-284
-28	-88	42
-27	228	-228
-26	-84	2
-25	338	-306
-24	-80	-79
-23	-77	-9
-22	-83	-13
-21	465	462
-20	-81	-138
-19	280	260
-18	-87	19
-17	844	-849
-16	197	266
-15	517	-534
-14	-57	15
-13	204	230
-12	1393	-1362
-11	-70	-33
-10	146	-180
-9	1076	1051
-8	935	1008
-7	1053	1064
-6	1111	1078
-5	239	-216
-4	410	-370
-3	1278	-1252
-2	892	805
-1	790	806

H= 4, K= 4

L	FO	FC
0	235	-170
1	551	-514
2	415	439
3	760	-732
4	212	-216
5	178	163
6	190	-193
7	1319	1339
8	155	-190
9	270	-260
10	223	208
11	517	-519
12	452	447
13	-78	29
14	833	-831
15	451	-453
16	312	-325
17	-82	-28
18	163	153
19	746	705
20	162	133
21	-82	21
22	146	-98
-29	-99	100
-28	233	-377
-27	469	-457
-26	-82	48
-25	-79	122
-24	-82	-73
-23	522	529
-22	222	-220
-21	398	403
-20	331	340
-19	1397	-1400
-18	521	511
-17	503	-495
-16	396	-383
-15	709	679
-14	1312	-1319
-13	-67	96
-12	227	263
-11	373	393
-10	194	146
-9	668	656
-8	277	-247
-7	844	-846
-6	434	370
-5	169	-154
-4	209	-108
-3	456	-438
-2	366	370
-1	120	-33

H= 6, K= 4

L	FO	FC
0	432	-420
1	1409	-1413
2	400	405
3	722	724
4	-63	-58
5	726	726
6	532	543
7	130	-170
8	501	463
9	692	-698
10	152	225
11	168	-191
12	497	-497
13	208	-189
14	169	-137
15	-80	53
16	-81	3
17	340	321
18	-83	24
19	-86	47
20	-85	-25
-30	142	-176
-29	518	-510
-28	-84	-99
-27	203	194
-26	-82	21
-25	657	648
-24	-82	121
-23	182	160
-22	-80	68
-21	630	-657
-20	207	156
-19	545	-551
-18	-75	-77
-17	596	511
-16	204	-168
-15	583	575
-14	214	-215
-13	-67	-62
-12	843	841
-11	-66	76
-10	482	442
-9	218	-208
-8	567	-515
-7	474	-461
-6	820	-851
-5	-70	-17
-4	255	264
-3	1244	1241
-2	519	-491
-1	657	-650

H= 8, K= 4

L	FO	FC
0	-72	-8
1	296	291
2	169	-154
3	570	562
4	221	232
5	157	131
6	-80	121
7	493	-490
8	-81	24
9	-81	21
10	-79	-11
11	235	220
12	307	-298
13	-81	16
14	323	317
15	236	227
16	211	192
-29	126	-140
-28	368	379
-27	502	492
-26	-79	115
-25	-77	17
-24	126	133
-23	301	-324
-22	201	161
-21	598	-601
-20	236	-251
-19	784	786
-18	432	-440
-17	414	425
-16	-75	71
-15	452	-433

L	FO	FC
-14	961	943
-13	203	-188
-12	-70	99
-11	274	-270
-10	251	-239
-9	716	-709
-8	131	122
-7	560	562
-6	-69	6
-5	654	655
-4	-59	19
-3	-69	-52
-2	379	-380
-1	549	-574

H= 10, K= 4

L	FO	FC
0	309	305
1	375	380
2	160	-161
3	274	-279
4	-81	51
5	365	-363
6	169	-168
7	-78	-66
8	221	-219
9	416	420
10	274	-279
11	159	130
12	198	215
-29	352	344
-28	179	118
-27	-81	-63
-26	-80	37
-25	411	-423
-24	-80	-113
-23	298	-281
-22	-80	-76
-21	543	537
-20	308	-310
-19	693	703
-18	-79	5
-17	478	-478
-16	295	293
-15	511	-490
-14	270	247
-13	182	148
-12	635	-625
-11	-75	-47
-10	243	-236
-9	-75	40
-8	398	391
-7	300	302
-6	323	319
-5	-77	112
-4	166	-195
-3	482	-493
-2	275	281
-1	-78	50

H= 12, K= 4

L	FO	FC
0	-80	64
1	-82	-74
2	-82	64
3	580	-589
4	-85	-89
5	174	-154
6	-87	-96
7	431	433
-27	528	-527
-26	177	-192
-25	172	-203
-24	-85	-115
-23	421	419
-22	-85	-132
-21	694	673
-20	-84	124

L	FO	FC
-19	580	-585
-18	307	300
-17	350	-358
-16	-82	-13
-15	176	194
-14	450	-430
-13	-81	102
-12	120	-76
-11	-80	117
-10	-81	-14
-9	296	321
-8	143	-88
-7	-81	-53
-6	-82	62
-5	183	-162
-4	-82	-53
-3	-81	0
-2	164	154
-1	413	416

H= 14, K= 4

L	FO	FC
0	164	-199
-24	-37	111
-23	271	285
-22	-86	84
-21	166	-163
-20	213	218
-19	452	-448
-18	-83	6
-17	-82	55
-16	-83	-98
-15	212	193
-14	208	-222
-13	-83	-84
-12	243	250
-11	120	-60
-10	217	206
-9	-82	25
-8	246	-229
-7	229	-222
-6	203	-188
-5	-83	-64
-4	150	182
-3	462	470
-2	125	-92
-1	-85	18

H= 1, K= 5

L	FO	FC
0	636	601
1	622	664
2	392	457
3	113	-163
4	526	-565
5	775	-730
6	140	-83
7	-68	-4
8	471	454
9	536	567
10	193	-219
11	217	258
12	151	162
13	472	489
14	370	-386
15	337	-345
16	-77	40
17	278	-287
18	-84	75
19	829	-825
20	-101	372
21	-89	161
22	-94	-300
23	531	538
24	-107	-97
25	218	-209
-27	-86	-104
-26	209	-213

L	FO	FC
-25	372	-361
-24	204	-207
-23	457	-437
-22	-82	110
-21	164	165
-20	-80	47
-19	621	615
-18	126	172
-17	215	-195
-16	-73	-78
-15	522	-516
-14	107	-51
-13	284	282
-12	514	526
-11	423	425
-10	244	225
-9	491	-480
-8	355	-427
-7	2513	2452
-6	1324	-1274
-5	-67	-25
-4	228	178
-3	2335	-2282
-2	1535	1459
-1	574	501

H= 3, K= 5

L	FO	FC
0	96	-87
1	185	180
2	896	-878
3	1063	-1143
4	338	-320
5	441	-485
6	769	769
7	1490	1481
8	224	209
9	146	-114
10	260	-252
11	289	279
12	389	-378
13	350	372
14	124	113
15	305	-283
16	178	202
17	402	-371
18	-82	-27
19	370	363
20	-84	-32
21	318	335
22	175	-193
23	240	-224
-28	-94	-99
-27	335	-340
-26	-88	-88
-25	274	-290
-24	-96	16
-23	451	504
-22	269	373
-21	443	476
-20	421	-460
-19	849	-824
-18	-78	-31
-17	539	-531
-16	-71	127
-15	510	-503
-14	611	619
-13	342	315
-12	-65	-57
-11	97	-11
-10	-69	37
-9	603	569
-8	1022	-1012
-7	-67	59
-6	276	-282
-5	639	-679
-4	636	595
-3	222	-180

L	FO	FC
-2	251	-218
-1	502	-475

H= 5, K= 5

L	FO	FC
0	488	-470
1	702	-676
2	371	-374
3	309	-306
4	614	594
5	1032	1040
6	228	233
7	359	361
8	411	-411
9	770	-785
10	-76	-36
11	255	-275
12	137	-140
13	305	-294
14	324	319
15	-81	75
16	-79	20
17	-81	48
18	-83	-34
19	454	436
20	248	-232
21	-86	20
-29	273	-247
-28	131	87
-27	-82	-15
-26	277	271
-25	531	537
-24	284	299
-23	827	829
-22	120	-163
-21	188	-177
-20	172	-195
-19	998	-970
-18	110	-111
-17	344	335
-16	179	214
-15	738	776
-14	117	146
-13	-67	-38
-12	476	-488
-11	601	-564
-10	238	-190
-9	768	711
-8	198	193
-7	1158	-1155
-6	626	672
-5	212	-196
-4	-69	-58
-3	1099	1111
-2	779	-784
-1	134	-113

H= 7, K= 5

L	FO	FC
0	160	150
1	334	-347
2	734	726
3	1256	1306
4	294	304
5	622	645
6	381	-368
7	842	-857
8	144	-144
9	-80	19
10	-81	35
11	177	-150
12	115	104
13	202	-201
14	-81	-75
15	140	147
16	138	-93
17	194	194
-29	358	-359

L	FO	FC
-28	-87	166
-27	435	458
-26	-83	116
-25	436	438
-24	-81	24
-23	563	-553
-22	408	-399
-21	639	-658
-20	333	306
-19	389	404
-18	-78	-120
-17	319	311
-16	-74	-79
-15	617	641
-14	322	-296
-13	-71	-115
-12	128	130
-11	-68	-6
-10	-67	7
-9	291	-291
-8	816	779
-7	328	-349
-6	274	281
-5	833	805
-4	629	-627
-3	471	448
-2	245	-212
-1	460	-463

H= 9, K= 5

L	FO	FC
0	258	277
1	218	208
2	328	324
3	-80	88
4	179	-149
5	355	-339
6	154	-138
7	269	-261
8	150	175
9	271	267
10	-80	-8
11	187	160
12	-83	16
13	191	173
14	251	-219
-29	225	223
-28	-82	-9
-27	-80	30
-26	157	-154
-25	319	-316
-24	250	-255
-23	636	-655
-22	-79	26
-21	229	-217
-20	165	124
-19	812	827
-18	-81	-26
-17	-78	-70
-16	259	-265
-15	651	-643
-14	-76	-31
-13	124	50
-12	556	560
-11	331	329
-10	283	306
-9	753	-758
-8	118	-110
-7	658	671
-6	555	-546
-5	238	233
-4	270	-255
-3	764	-763
-2	299	304
-1	124	72

H= 11, K=

L	FO	FC
0	-80	-3
1	281	270
2	305	-306
3	626	-644
4	170	-162
5	601	-593
6	218	208
7	434	435
8	162	139
9	-84	106
-27	306	-322
-26	-83	-103
-25	532	-535
-24	-81	-3
-23	379	392
-22	363	366
-21	807	822
-20	274	-296
-19	182	-193
-18	-80	-45
-17	399	-385
-16	-81	22
-15	312	-294
-14	245	247
-13	182	161
-12	-80	77
-11	-80	18
-10	-80	57
-9	-79	-34
-8	432	-448
-7	212	187
-6	216	-214
-5	-81	-103
-4	198	183
-3	161	-139
-2	-82	92
-1	-80	60

H= 13, K= 5

L	FO	FC
0	232	-247
1	262	-263
2	161	-171
3	229	-232
-25	244	233
-24	174	194
-23	540	543
-22	-84	4
-21	225	238
-20	-84	-93
-19	547	-560
-18	-82	-13
-17	-81	-85
-16	136	114
-15	271	277
-14	-79	5
-13	-81	37
-12	261	-264
-11	197	-204
-10	-82	-99
-9	403	421
-8	-81	57
-7	209	-203
-6	231	203
-5	210	-240
-4	204	222
-3	489	506
-2	128	-122
-1	227	199

H= 15, K= 5

L	FO	FC
-18	-86	14
-17	169	145
-16	-80	-34
-15	192	156
-14	179	-179
-13	-85	-106

L	FO	FC
-12	-65	-70
-11	-85	-3
-10	-86	-2
-9	-86	55
-8	288	311
-7	198	-189
-6	184	153

H= 0, K= 6

L	FO	FC
0	1641	1600
1	1043	948
2	-70	70
3	657	-615
4	1508	-1469
5	1763	-1815
6	857	-874
7	744	-730
8	-64	25
9	840	778
10	135	222
11	280	306
12	142	142
13	396	-389
14	-73	-89
15	399	421
16	359	-364
17	281	282
18	388	399
19	248	-250
20	305	280
21	460	-465
22	287	-275
23	145	165
24	118	1
25	293	291
26	318	-302

H= 2, K= 6

L	FO	FC
0	-67	56
1	683	681
2	554	-547
3	870	-838
4	342	-351
5	144	115
6	158	-161
7	812	827
8	1263	1259
9	-68	-59
10	-69	-5
11	703	-718
12	433	-429
13	-75	19
14	196	-175
15	288	288
16	174	172
17	410	-388
18	272	302
19	212	-288
20	159	-241
21	-85	117
22	278	-295
23	460	473
24	-101	-191
-27	209	-179
-26	240	-233
-25	-79	-9
-24	-85	182
-23	578	555
-22	267	264
-21	145	165
-20	294	298
-19	-77	-53
-18	250	-221
-17	420	-413
-16	216	-215
-15	140	124

L	FO	FC
-14	195	234
-13	-68	-87
-12	728	745
-11	1395	-1474
-10	115	103
-9	658	-635
-8	1888	-1908
-7	1531	1450
-6	-69	2
-5	300	354
-4	746	732
-3	872	-916
-2	877	844
-1	657	713

H= 4, K= 6

L	FO	FC
0	958	-991
1	579	-575
2	218	-225
3	-65	87
4	803	799
5	962	975
6	726	738
7	649	665
8	-73	130
9	620	-599
10	428	-409
11	316	-331
12	307	-326
13	567	578
14	209	205
15	278	-268
16	468	464
17	421	-414
18	240	-219
19	-84	96
20	273	-254
21	309	314
-28	-86	-28
-27	127	-196
-26	313	322
-25	267	276
-24	-81	20
-23	332	334
-22	346	350
-21	382	-365
-20	396	-392
-19	406	-413
-18	677	-555
-17	447	402
-16	533	530
-15	726	731
-14	440	414
-13	695	-651
-12	295	-293
-11	-67	-108
-10	463	-483
-9	809	834
-8	162	-135
-7	302	-359
-6	598	583
-5	1099	-1093
-4	1123	1159
-3	773	-812
-2	202	213
-1	271	265

H= 6, K= 6

L	FO	FC
0	285	-311
1	810	-827
2	503	467
3	705	773
4	525	527
5	325	334
6	-77	105
7	765	-759

L	FO	FC
8	924	-936
9	184	-212
10	-82	-84
11	475	455
12	236	214
13	-81	40
14	-80	23
15	128	-148
16	-82	-52
17	181	193
18	-86	-101
-28	211	209
-27	142	145
-26	364	360
-25	203	206
-24	171	-190
-23	631	-644
-22	316	-319
-21	353	-340
-20	198	-227
-19	-78	13
-18	219	182
-17	352	376
-16	161	172
-15	160	138
-14	-72	-40
-13	193	193
-12	283	-292
-11	914	916
-10	286	-288
-9	755	761
-8	1085	1088
-7	858	-853
-6	127	140
-5	408	-411
-4	262	-278
-3	899	879
-2	753	-728
-1	171	-183

H= 8, K= 6

L	FO	FC
0	677	674
1	479	469
2	161	150
3	-80	129
4	339	-338
5	463	-459
6	208	-226
7	419	-405
8	-80	-53
9	-79	89
10	-79	92
11	220	194
12	-82	143
13	193	-201
14	-84	-79
15	147	143
-28	-83	14
-27	183	201
-26	303	-294
-25	261	-252
-24	-80	38
-23	390	-369
-22	340	-338
-21	-80	128
-20	147	132
-19	195	175
-18	523	529
-17	171	-149
-16	295	-280
-15	483	-499
-14	358	-365
-13	463	464
-12	158	188
-11	314	302
-10	558	574
-9	1052	-1033
-8	293	296
-7	313	-310
-6	651	-638
-5	902	904
-4	1003	-1000
-3	496	506
-2	-75	-61
-1	189	-215

H= 10, K= 6

L	FO	FC
0	186	195
1	374	367
2	145	-148
3	242	-267
4	271	-266
5	281	-300
6	-81	-114
7	265	244
8	503	509
9	149	138
10	161	131
11	283	-274
-27	-84	-90
-26	346	-346
-25	183	-202
-24	117	120
-23	395	415
-22	296	286
-21	264	287
-20	131	149
-19	-81	106
-18	237	-210
-17	318	-315
-16	351	-336
-15	-80	87
-14	116	90
-13	197	227
-12	477	471
-11	619	-629
-10	317	312
-9	829	-826
-8	759	-752
-7	343	338
-6	176	-197
-5	239	229
-4	-80	76
-3	229	-245
-2	238	282
-1	-81	35

H= 12, K= 6

L	FO	FC
0	322	-314
1	128	-108
2	160	-189
3	258	-232
4	132	124
5	216	197
-25	-84	49
-24	123	44
-23	382	365
-22	280	260
-21	-33	-33
-20	128	-119
-19	250	-213
-18	415	-399
-17	-81	63
-16	147	160
-15	365	395
-14	251	263
-13	179	-162
-12	-81	-80
-11	202	-195
-10	178	-166
-9	407	424
-8	156	-152
-7	243	247
-6	156	161
-5	330	-336
-4	484	475
-3	246	-232
-2	165	129
-1	195	184

H= 14, K= 6

L	FO	FC
-21	-87	-113
-20	-86	-21
-19	168	-130
-18	-85	27
-17	-84	34
-16	-85	140
-15	-84	-32
-14	-84	0
-13	-84	-120
-12	211	-214
-11	239	234
-10	252	-251
-9	566	561
-8	394	397
-7	232	-214
-6	227	235
-5	250	-244
-4	-88	-36
-3	156	155
-2	232	-222

H= 1, K= 7

L	FO	FC
0	756	-718
1	178	-187
2	277	269
3	144	100
4	776	-769
5	696	-670
6	253	200
7	1438	1450
8	333	-322
9	879	911
10	146	-159
11	527	-521
12	165	191
13	125	-102
14	112	-116
15	207	234
16	148	-98
17	147	125
18	-82	71
19	609	-579
20	-83	-19
21	423	-425
22	-84	-116
23	-84	49
24	-85	-48
-26	-83	0
-25	119	62
-24	175	161
-23	-81	111
-22	-78	-71
-21	548	551
-20	245	-258
-19	280	-269
-18	404	411
-17	377	-370
-16	331	-340
-15	496	491
-14	277	-322
-13	508	492
-12	690	729
-11	269	-263
-10	110	-109
-9	1398	-1402
-8	104	-147
-7	992	982
-6	285	250
-5	1062	1060
-4	458	521
-3	437	438
-2	115	-98
-1	318	-336

H= 3, K= 7

L	FO	FC
0	265	292
1	458	-441
2	214	239
3	116	140
4	184	-159
5	236	272
6	121	-154
7	877	891
8	154	176
9	706	-715
10	304	308
11	340	-351
12	631	-628
13	527	529
14	119	138
15	658	654
16	413	406
17	399	-413
18	249	-255
19	431	-429
20	-86	62
21	446	450
22	-90	52
-27	232	217
-26	-83	-52
-25	242	226
-24	-81	57
-23	-79	80
-22	158	93
-21	274	-278
-20	-83	93
-19	668	-692
-18	121	-143
-17	-77	51
-16	-75	-42
-15	589	596
-14	288	246
-13	347	-347
-12	167	-184
-11	1372	-1376
-10	206	-208
-9	791	793
-8	231	233
-7	1911	1954
-6	-65	-5
-5	522	-541
-4	988	1005
-3	182	133
-2	273	-271
-1	333	-304

H= 5, K= 7

L	FO	FC
0	366	352
1	-68	23
2	568	-553
3	141	-100
4	363	374
5	669	666
6	146	170
7	1133	-1141
8	265	257
9	940	-955
10	-81	-24
11	497	508
12	130	-109
13	248	215
14	136	129
15	240	-231
16	-82	39

L	FO	FC
17	159	-148
18	-84	-71
19	318	289
-27	-84	92
-26	-81	42
-25	-79	34
-24	128	-144
-23	-78	-40
-22	146	137
-21	649	-645
-20	288	315
-19	249	273
-18	466	-472
-17	598	596
-16	365	375
-15	476	-478
-14	290	308
-13	459	-447
-12	738	-711
-11	-69	84
-10	-70	37
-9	1080	1083
-8	-68	2
-7	445	-420
-6	277	-268
-5	501	-525
-4	228	-251
-3	474	-456
-2	94	-19
-1	198	184

H= 7, K= 7

L	FO	FC
0	-75	-40
1	438	424
2	340	-351
3	125	95
4	-79	-40
5	123	-98
6	-81	117
7	574	-582
8	-81	49
9	211	235
10	176	-187
11	-83	144
12	265	249
13	166	-150
14	-83	-59
15	326	-308
16	237	-209
-28	-84	-68
-27	202	-200
-26	-82	-28
-25	265	-239
-24	-80	-2
-23	122	-122
-22	-79	47
-21	-82	118
-20	123	-95
-19	396	387
-18	-79	1
-17	119	132
-16	-77	24
-15	294	-279
-14	-76	-11
-13	-75	107
-12	136	139
-11	933	964
-10	-73	42
-9	273	-252
-8	-73	25
-7	1711	-1704
-6	283	233
-5	150	132
-4	685	-694
-3	214	225
-2	276	246
-1	400	394

H= 9, K= 7

L	FO	FC
0	250	-248
1	-80	34
2	222	238
3	154	155
4	132	-183
5	387	-381
6	-80	-71
7	374	365
8	-82	-106
9	478	457
10	-84	23
11	-86	-186
12	-86	102
-27	-84	-118
-26	122	-111
-25	-81	-73
-24	158	143
-23	-78	-31
-22	-79	-77
-21	411	403
-20	326	-323
-19	-80	-63
-18	397	414
-17	453	-459
-16	295	-313
-15	307	316
-14	401	-423
-13	724	724
-12	530	528
-11	-79	83
-10	-79	157
-9	1346	-1338
-8	232	-249
-7	-79	-92
-6	-73	-2
-5	475	474
-4	316	346
-3	312	327
-2	214	210
-1	-79	-51

H= 11, K= 7

L	FO	FC
0	-80	14
1	210	-213
2	166	171
3	-82	-61
4	-81	-45
5	-84	-47
6	-85	-124
7	342	348
-25	-84	119
-24	-82	-18
-23	-82	102
-22	-80	-24
-21	-80	-12
-20	153	162
-19	256	-290
-18	-79	-4
-17	-79	-100
-16	-79	-39
-15	496	509
-14	-80	80
-13	-79	7
-12	120	-56
-11	612	-633
-10	-81	-93
-9	-81	-31
-8	-81	-72
-7	800	811
-6	255	-243
-5	-80	-5
-4	337	343
-3	-80	34
-2	-79	-33

L	FO	FC
-1	191	-180

H= 13, K= 7

L	FO	FC
0	171	165
1	-87	3
-22	-86	24
-21	243	-224
-20	297	302
-19	-84	0
-18	200	-217
-17	133	190
-15	136	130
-15	189	-169
-14	245	231
-13	303	-283
-12	190	-170
-11	135	-162
-10	-83	-77
-9	621	633
-8	-84	61
-7	214	217
-6	-85	37
-5	255	-259
-4	143	-107
-3	235	-240
-2	-86	-120
-1	124	92

H= 0, K= 8

L	FO	FC
0	1309	-1290
1	246	248
2	152	170
3	833	-852
4	992	982
5	393	-400
6	397	370
7	249	274
8	474	-501
9	496	495
10	264	-251
11	-73	-25
12	241	-262
13	422	-404
14	-77	25
15	-79	57
16	-81	-104
17	129	70
18	468	455
19	-81	-128
20	185	-164
21	134	-125
22	206	-204
23	149	-122
24	343	338

H= 2, K= 8

L	FO	FC
0	214	-228
1	654	-676
2	1175	1180
3	127	100
4	-67	134
5	-68	81
6	249	-258
7	275	282
8	111	-60
9	719	739
10	228	235
11	689	-691
12	211	-187
13	-78	-74
14	-81	-20
15	775	772
16	-83	65
17	304	-293
18	-81	-100

L	FO	FC
19	159	-177
20	444	-429
21	-86	71
22	237	225
-25	-81	-17
-24	232	-210
-23	140	156
-22	349	-309
-21	218	216
-20	370	374
-19	-80	-20
-18	-80	104
-17	566	-583
-16	-73	-88
-15	822	836
-14	-74	-30
-13	142	147
-12	245	217
-11	1199	-1215
-10	305	-292
-9	380	395
-8	192	170
-7	708	725
-6	765	775
-5	351	390
-4	216	197
-3	112	117
-2	1378	-1379
-1	699	-699

H= 4, K= 8

L	FO	FC
0	520	508
1	318	-349
2	107	-123
3	450	434
4	699	-702
5	485	499
6	320	-329
7	-75	22
8	527	524
9	539	-559
10	325	340
11	-83	-133
12	148	128
13	463	472
14	124	-6
15	-81	-85
16	165	130
17	260	-267
18	364	-314
19	-86	89
20	-87	33
-26	206	-215
-25	262	254
-24	442	-436
-23	-81	44
-22	248	220
-21	-81	-82
-20	378	379
-19	245	-262
-18	674	-662
-17	132	155
-16	127	-110
-15	120	107
-14	-75	-20
-13	697	-711
-12	129	158
-11	163	-150
-10	-71	25
-9	677	676
-8	486	484
-7	334	343
-6	154	-150
-5	127	-134
-4	544	-581
-3	729	-740
-2	445	-422

L	FO	FC
-1	-67	39

H= 6, K= 8

L	FO	FC
0	408	385
1	483	494
2	1240	-1221
3	220	193
4	431	-419
5	-79	39
6	325	343
7	221	-206
8	199	172
9	453	-447
10	201	-188
11	374	351
12	-81	99
13	-82	-7
14	-83	-18
15	508	-480
16	-87	-38
17	136	133
-27	170	-171
-26	232	-240
-25	-83	87
-24	308	283
-23	-82	-79
-22	499	505
-21	265	-277
-20	282	-279
-19	156	-136
-18	-82	-125
-17	473	460
-16	-79	34
-15	608	-607
-14	-76	47
-13	-75	-6
-12	-76	-90
-11	900	913
-10	125	142
-9	173	-138
-8	-73	-109
-7	316	-295
-6	344	-343
-5	382	-414
-4	175	-166
-3	338	-371
-2	1054	1057
-1	402	411

H= 8, K= 8

L	FO	FC
0	406	-410
1	175	194
2	172	-134
3	154	-165
4	322	324
5	226	-196
6	254	240
7	-81	-65
8	142	-144
9	201	165
10	212	-178
11	158	151
12	140	-76
13	176	-161
-26	137	97
-25	208	-189
-24	407	405
-23	-80	-82
-22	-77	-29
-21	-80	-98
-20	339	-357
-19	185	185
-18	465	478
-17	-80	9
-16	137	109
-15	154	-171
-14	-80	-5
-13	439	480
-12	194	-170
-11	502	504
-10	-79	52
-9	576	-571
-8	462	-483
-7	715	-700
-6	-78	-24
-5	175	156
-4	756	746
-3	620	602
-2	580	595
-1	-80	-96

H= 10, K= 8

L	FO	FC
0	290	-279
1	229	-257
2	466	474
3	117	-126
4	203	194
5	178	-140
6	-86	-157
7	-84	58
8	-87	-135
9	306	293
-25	-85	-101
-24	140	-150
-23	-83	-13
-22	406	-416
-21	322	325
-20	230	184
-19	132	175
-18	216	214
-17	463	-471
-16	-80	-35
-15	571	575
-14	-83	-155
-13	219	218
-12	-82	3
-11	802	-796
-10	134	-184
-9	179	-160
-8	-81	-33
-7	261	255
-6	180	141
-5	212	244
-4	226	200
-3	301	302
-2	354	-363
-1	172	-151

H= 12, K= 8

L	FO	FC
0	205	244
1	-86	-119
2	126	157
3	-37	24
-23	-86	92
-22	-84	-8
-21	151	132
-20	441	454
-19	-84	-83
-18	270	-258
-17	-82	23
-16	-84	-111
-15	-81	27
-14	-82	5
-13	267	-271
-12	-82	94
-11	289	-292
-10	-82	-64
-9	193	200
-8	209	227
-7	429	424
-6	-84	31
-5	-83	84
-4	313	-321
-3	286	-258
-2	306	-329
-1	-85	31

H= 14, K= 8

L	FO	FC
-16	-85	-18
-15	321	-297
-14	-87	86
-13	196	-208
-12	-86	28
-11	327	329
-10	-87	93
-9	279	274
-8	-86	24

H= 1, K= 9

L	FO	FC
0	1509	-1565
1	105	-117
2	591	598
3	-68	79
4	564	579
5	815	-823
6	537	-538
7	-73	50
8	687	-695
9	467	440
10	294	322
11	-78	-102
12	149	93
13	-80	115
14	-80	11
15	255	-257
16	174	171
17	-81	65
18	163	149
19	417	-421
20	454	-444
21	210	225
22	132	-100
-24	-84	-94
-23	144	-149
-22	478	-462
-21	415	387
-20	294	302
-19	-79	126
-18	-79	53
-17	370	-374
-16	-80	77
-15	-78	-114
-14	148	191
-13	555	-570
-12	139	169
-11	-73	-58
-10	247	-268
-9	281	-275
-8	-71	-59
-7	899	906
-6	649	661
-5	390	418
-4	888	904
-3	-68	3
-2	759	-785
-1	-63	49

H= 3, K= 9

L	FO	FC
0	944	975
1	112	-42
2	465	474
3	105	109
4	286	-297
5	264	235
6	296	-272
7	892	878
8	-79	-83
9	-79	-22
10	306	279
11	-81	-74
12	-82	-72
13	482	-472
14	-81	-59
15	136	-128
16	-81	-20
17	355	-349
18	-85	-85
19	-85	38
20	293	-293
-25	129	-157
-24	451	-453
-23	275	294
-22	141	-94
-21	394	415
-20	474	461
-19	464	-504
-18	198	-176
-17	-81	-44
-16	342	-340
-15	246	-243
-14	-78	-102
-13	-78	111
-12	-76	-78
-11	135	-142
-10	437	-432
-9	537	603
-8	750	770
-7	300	333
-6	651	668
-5	942	-903
-4	387	-383
-3	134	-125
-2	355	-411
-1	286	-274

H= 5, K= 9

L	FO	FC
0	1253	1258
1	-76	-35
2	369	-360
3	149	-134
4	779	-797
5	773	775
6	287	303
7	219	203
8	693	538
9	339	-343
10	283	-272
11	-80	80
12	233	-203
13	151	-180
14	115	13
15	-84	30
16	-85	-42
17	-86	-63
-26	685	-653
-25	103	171
-24	-84	32
-23	330	337
-22	702	710
-21	402	-388
-20	228	-235
-19	329	-311
-18	239	-255
-17	237	250
-16	117	-94
-15	122	-113
-14	-79	-56
-13	633	642
-12	-77	-110
-11	290	319
-10	-75	34
-9	407	401
-8	-74	-57
-7	564	-551

L	FO	FC
-6	331	-348
-5	423	-408
-4	722	-738
-3	248	-243
-2	200	197
-1	211	-222

H= 7, K= 9

L	FO	FC
0	630	-625
1	-81	16
2	701	-682
3	-81	68
4	169	189
5	-80	39
6	283	294
7	443	-450
8	-81	84
9	-80	-24
10	233	-244
11	-82	-72
12	-83	6
13	256	227
14	-86	33
-26	129	-81
-25	218	235
-24	481	499
-23	156	-148
-22	231	215
-21	479	-458
-20	382	-397
-19	219	227
-18	128	153
-17	118	-52
-16	289	284
-15	228	219
-14	151	182
-13	-80	-93
-12	143	117
-11	224	212
-10	428	437
-9	225	-191
-8	537	-544
-7	372	-405
-6	708	-718
-5	617	614
-4	377	383
-3	184	150
-2	777	780
-1	-80	-17

H= 9, K= 9

L	FO	FC
0	666	-662
1	-80	-8
2	-81	111
3	115	129
4	327	342
5	348	-342
6	-83	-66
7	219	-216
8	284	-274
9	235	191
10	135	138
-25	169	-127
-24	-84	35
-23	328	-325
-22	477	-493
-21	233	230
-20	-81	68
-19	328	351
-18	130	105
-17	221	-253
-16	-79	101
-15	-80	81
-14	-80	6
-13	362	-366
-12	-81	26

L	FO	FC
-11	236	-244
-10	-81	-57
-9	373	-373
-8	132	-120
-7	373	355
-6	290	264
-5	346	321
-4	597	597
-3	-82	64
-2	-81	-14
-1	-81	97

H= 11, K= 9

L	FO	FC
0	174	141
1	-84	-60
2	349	341
3	-87	-95
4	-87	-33
-23	-84	32
-22	289	-301
-21	401	465
-20	425	462
-19	-82	-51
-18	-81	27
-17	-81	17
-16	350	-344
-15	159	-155
-14	209	-225
-13	-80	-42
-12	-79	6
-11	122	-150
-10	257	-260
-9	147	113
-8	246	225
-7	330	317
-6	323	333
-5	236	-243
-4	119	-115
-3	125	-79
-2	354	-358
-1	-84	-7

H= 13, K= 9

L	FO	FC
-18	-85	-36
-17	-87	122
-16	-86	-72
-15	190	-173
-14	-85	-30
-13	146	154
-12	-85	20
-11	155	97
-10	-85	59
-9	246	210
-8	-87	120
-7	-87	-45
-6	-88	-94
-5	-87	-135
-4	420	-405

H= 0, K= 10

L	FO	FC
0	1132	-1196
1	752	775
2	-72	-1
3	415	395
4	820	823
5	156	-151
6	442	-443
7	335	-335
8	384	-384
9	141	-158
10	528	536
11	365	376
12	149	-106
13	232	223
14	117	-93

L	FO	FC
15	171	171
16	-81	102
17	369	-378
18	182	-190
19	481	-430
20	-83	-20
21	-84	22
22	238	-246

H= 2, K= 10

L	FO	FC
0	-72	81
1	220	214
2	402	410
3	744	-751
4	326	331
5	219	-189
6	317	-322
7	-79	90
8	-78	-3
9	492	472
10	333	321
11	456	442
12	379	-383
13	-82	47
14	204	-213
15	473	-438
16	-82	38
17	454	-437
18	218	233
19	-38	103
20	466	-452
-23	155	136
-22	341	-349
-21	226	202
-20	441	443
-19	165	211
-18	158	-212
-17	428	-434
-16	-81	0
-15	555	-606
-14	256	262
-13	-78	-9
-12	490	508
-11	484	499
-10	438	-439
-9	640	639
-8	196	-191
-7	145	146
-6	561	560
-5	322	-349
-4	255	-258
-3	753	-760
-2	377	-391
-1	302	309

H= 4, K= 10

L	FO	FC
0	695	719
1	461	-473
2	344	343
3	435	-397
4	538	-511
5	-79	52
6	261	250
7	414	435
8	395	401
9	331	293
10	400	-402
11	277	-283
12	-81	-109
13	257	-250
14	138	158
15	295	-276
16	-84	11
17	218	200
-24	233	-233
-23	422	419

L	FO	FC
-22	243	237
-21	200	168
-20	-82	108
-19	590	-576
-18	-80	59
-17	650	-637
-16	199	-184
-15	-80	23
-14	240	244
-13	301	342
-12	334	339
-11	471	506
-10	653	-672
-9	-77	-88
-8	-76	-58
-7	294	-215
-6	253	254
-5	-75	-83
-4	516	-540
-3	-75	79
-2	217	-230
-1	539	544

H= 6, K= 10

L	FO	FC
0	211	188
1	388	-382
2	452	-455
3	509	531
4	351	-328
5	378	373
6	386	380
7	-80	52
8	-80	10
9	318	-293
10	434	-443
11	374	-537
12	-80	144
13	177	-125
14	172	168
-24	166	166
-23	-83	-32
-22	408	456
-21	254	-242
-20	556	-558
-19	348	-345
-18	-79	80
-17	203	214
-16	127	64
-15	525	536
-14	-80	-7
-13	147	111
-12	233	-243
-11	213	-236
-10	264	283
-9	367	-346
-8	169	169
-7	231	-215
-6	445	-449
-5	-80	115
-4	-76	-15
-3	583	590
-2	334	337
-1	281	-253

H= 8, K= 10

L	FO	FC
0	458	-470
1	312	334
2	233	-237
3	352	324
4	394	406
5	-80	-18
6	151	-140
7	201	-219
8	241	-254
9	159	-160
10	198	165

L	FO	FC
11	-85	115
-24	161	171
-23	385	-373
-22	179	-172
-21	240	-209
-20	-81	-123
-19	358	349
-18	160	-183
-17	494	499
-16	146	136
-15	-80	102
-14	-80	-72
-13	226	-229
-12	271	-277
-11	371	-367
-10	590	600
-9	-82	60
-8	-81	44
-7	213	231
-6	386	-373
-5	-82	99
-4	469	482
-3	190	-193
-2	351	356
-1	460	-447
H=	10, K=	10
0	124	-104
1	135	164
2	134	123
3	241	-225
4	252	228
5	255	-245
6	-87	-105
-22	432	-432
-21	242	202
-20	421	413
-19	391	410
-18	-84	62
-17	-83	-87
-16	170	-152
-15	499	-500
-14	186	-159
-13	163	-184
-12	247	226
-11	183	169
-10	-82	-86
-9	270	264
-8	146	-183
-7	129	149
-6	138	135
-5	145	-86
-4	124	-84
-3	315	-285
-2	-82	-84
-1	-83	106
H=	12, K=	10
-18	-86	70
-17	360	-328
-16	172	-184
-15	184	-188
-14	-87	15
-13	-86	79
-12	318	295
-11	199	192
-10	222	-238
-9	-85	-15
-8	-85	-84
-7	-86	-31
-6	237	227
-5	-87	-29
-4	258	-226
-3	129	60
-2	320	-332

L	FO	FC
H=	1, K=	11
0	166	-211
1	-76	-112
2	259	248
3	168	189
4	-76	-22
5	396	-386
6	337	-310
7	-79	-28
8	253	233
9	171	-186
10	548	558
11	336	389
12	704	-690
13	306	289
14	534	-511
15	315	-305
16	-82	33
17	-84	-53
18	418	413
19	-85	-121
20	-86	-44
-21	256	248
-20	410	410
-19	239	266
-18	-80	-68
-17	128	167
-16	224	-222
-15	364	-352
-14	409	-413
-13	403	-376
-12	473	489
-11	-80	70
-10	638	710
-9	112	-18
-8	687	-727
-7	195	206
-6	729	-759
-5	282	-291
-4	331	357
-3	204	-242
-2	-76	-32
-1	393	415
H=	3, K=	11
0	126	115
1	255	255
2	162	175
3	211	-186
4	154	-173
5	297	-304
6	536	556
7	125	115
8	622	600
9	-82	56
10	447	-440
11	197	229
12	547	-546
13	332	-280
14	277	292
15	432	-398
16	239	287
17	-86	85
-22	126	-14
-21	291	298
-20	-82	73
-19	-81	-33
-18	532	-539
-17	-80	-105
-16	220	-236
-15	519	-476
-14	533	609
-13	252	241
-12	1005	1038
-11	564	545
-10	591	-600

L	FO	FC
-9	240	-237
-8	497	-520
-7	175	-106
-6	311	311
-5	-79	-137
-4	121	113
-3	471	474
-2	193	-208
-1	114	-94
H=	5, K=	11
0	229	241
1	153	110
2	-80	-71
3	296	-309
4	-80	-65
5	267	300
6	306	319
7	195	174
8	124	-101
9	241	225
10	729	-738
11	306	-278
12	355	300
13	292	-269
14	491	475
15	196	184
-23	188	173
-22	-84	76
-21	223	-225
-20	522	-527
-19	448	-402
-18	-83	-122
-17	255	-247
-16	348	345
-15	340	305
-14	536	555
-13	320	333
-12	230	-214
-11	-81	-46
-10	680	-705
-9	-81	55
-8	276	275
-7	172	-150
-6	524	551
-5	120	81
-4	240	-239
-3	198	174
-2	165	-136
-1	196	-195
H=	7, K=	11
0	-81	59
1	157	-143
2	-82	-155
3	167	213
4	253	273
5	191	167
6	324	-293
7	164	-153
8	467	-456
9	-85	-19
10	-87	122
11	-88	-132
-23	214	-210
-22	-84	23
-21	289	-285
-20	132	-102
-19	-83	12
-18	400	409
-17	-80	59
-16	295	295
-15	431	413
-14	162	-174
-13	117	-1
-12	832	-839

L	FO	FC
-11	358	-348
-10	231	267
-9	-81	103
-8	538	544
-7	-82	-46
-6	338	-353
-5	-83	72
-4	305	-305
-3	341	-353
-2	337	311
-1	-81	-49
H=	9, K=	11
0	136	-107
1	-82	-8
2	-80	5
3	172	156
4	-84	82
5	213	-197
6	-83	-85
-21	170	98
-20	369	369
-19	353	368
-18	202	174
-17	281	303
-16	276	-286
-15	164	-164
-14	526	-540
-13	270	-257
-12	143	157
-11	-81	-22
-10	657	576
-9	-81	58
-8	194	-216
-7	-81	72
-6	531	-521
-5	157	-180
-4	140	121
-3	-81	-119
-2	143	151
-1	292	304
H=	11, K=	11
0	140	-141
-18	308	-312
-17	-87	-68
-16	375	-374
-15	323	-318
-14	-85	38
-13	124	-43
-12	644	645
-11	215	225
-10	-85	0
-9	141	-119
-8	353	-353
-7	-84	7
-6	-86	130
-5	-86	28
-4	190	189
-3	179	184
-2	187	-192
-1	-88	38
H=	0, K=	12
0	370	-384
1	327	-331
2	132	129
3	661	-656
4	140	-125
5	-80	-108
6	169	-204
7	291	298
8	-80	-62
9	125	-160
10	651	560

L	FO	FC
11	569	559
12	253	228
13	168	-178
14	510	-492
15	-80	43
16	399	-388
17	-82	5
18	335	333
19	-85	43
H=	2, K=	12
0	-80	-99
1	268	-283
2	387	395
3	322	-316
4	712	-695
5	653	660
6	-82	-63
7	122	-105
8	280	266
9	195	171
10	-81	11
11	-82	42
12	562	-568
13	165	-132
14	273	-263
15	-83	-33
16	316	280
17	-86	-37
-20	-86	153
-19	-85	115
-18	498	--508
-17	-83	32
-16	527	-510
-15	-79	16
-14	124	105
-13	205	-197
-12	840	856
-11	-81	-66
-10	150	146
-9	211	185
-8	469	-466
-7	242	-238
-6	183	186
-5	810	836
-4	946	935
-3	116	25
-2	367	-380
-1	165	-184
H=	4, K=	12
0	275	277
1	218	194
2	-80	14
3	410	402
4	-81	61
5	-80	62
6	194	207
7	252	-261
8	254	274
9	348	296
10	567	-552
11	324	-319
12	426	-419
13	-86	85
14	436	414
-21	-83	-51
-20	206	-208
-19	-84	73
-18	554	-594
-17	-82	-3
-16	361	365
-15	-80	42
-14	654	666
-13	262	-271
-12	208	-164

L	FO	FC
-11	501	519
-10	714	-720
-9	158	-160
-8	-81	15
-7	273	239
-6	-81	91
-5	117	65
-4	-81	79
-3	464	-472
-2	232	-229
-1	266	-270
H=	5, K=	12
0	138	142
1	237	222
2	337	-338
3	254	236
4	590	563
5	542	-540
6	-81	55
7	-82	-29
8	288	-281
9	-85	-68
10	134	-111
11	143	-45
-21	237	234
-20	194	-161
-19	-83	-29
-18	481	475
-17	-83	-68
-16	506	490
-15	138	-83
-14	-81	96
-13	-82	133
-12	555	-565
-11	125	129
-10	239	-302
-9	272	-221
-8	213	254
-7	-82	135
-6	-81	-64
-5	692	-723
-4	737	-742
-3	-81	-42
-2	194	195
-1	230	247
H=	8, K=	12
0	-81	-92
1	-81	46
2	131	-90
3	220	-220
4	-83	-75
5	163	-182
6	-85	-74
7	-86	113
-20	153	133
-19	-84	-8
-18	517	553
-17	-83	15
-16	146	-143
-15	-81	-18
-14	524	-551
-13	364	345
-12	126	-60
-11	360	-371
-10	641	643
-9	-80	31
-8	-80	108
-7	172	-193
-6	210	-206
-5	182	-188
-4	-81	-73
-3	322	297
-2	353	368
-1	395	404

L	FO	FC
H=	10, K=	12
0	175	-140
-17	-83	133
-16	534	-526
-15	192	121
-14	254	-216
-13	-84	-64
-12	477	469
-11	-87	-95
-10	238	231
-9	126	128
-8	271	-270
-7	227	-230
-6	-86	64
-5	384	381
-4	506	496
-3	134	103
-2	-85	-78
-1	-86	-82
H=	1, K=	13
0	375	-384
1	766	-769
2	424	436
3	464	-510
4	-83	40
5	150	175
6	298	303
7	452	443
8	-80	12
9	116	-129
10	164	161
11	-82	103
12	-84	103
13	-83	-40
14	310	-290
15	193	-172
16	340	-277
-18	-85	115
-17	-83	32
-16	297	-315
-15	205	224
-14	151	-128
-13	135	-112
-12	410	422
-11	195	136
-10	162	165
-9	197	-225
-8	421	-429
-7	406	-354
-6	300	339
-5	551	562
-4	147	157
-3	277	282
-2	393	-403
-1	163	-112
H=	3, K=	13
0	149	121
1	221	-173
2	381	372
3	-81	57
4	-80	35
5	501	477
6	275	-286
7	175	-148
8	419	405
9	186	-181
10	-83	57
11	127	95
12	448	-422
13	136	-111
14	-87	-58
-19	120	-4

L	FO	FC
-18	283	-302
-17	349	342
-16	126	92
-15	181	-165
-14	322	344
-13	-82	-143
-12	-80	-13
-11	-80	112
-10	163	-224
-9	174	-159
-8	-81	47
-7	388	374
-6	123	-137
-5	302	317
-4	120	-49
-3	253	-279
-2	560	-560
-1	601	-587
H=	5, K=	13
0	303	310
1	564	559
2	402	-397
3	528	536
4	-81	-41
5	-82	-117
6	220	-153
7	435	-433
8	-85	37
9	159	141
10	180	-173
11	-85	-2
-19	354	343
-18	187	-177
-17	-83	-77
-16	301	293
-15	298	-327
-14	135	132
-13	-80	32
-12	347	-343
-11	-82	-78
-10	147	-112
-9	156	103
-8	400	403
-7	248	269
-6	307	-296
-5	416	-442
-4	161	-138
-3	144	-169
-2	236	243
-1	-81	5
H=	7, K=	13
0	-83	22
1	270	245
2	347	-318
3	119	-109
4	150	-141
5	396	-406
6	137	146
7	-85	73
-18	250	238
-17	299	-294
-16	-83	-33
-15	-84	94
-14	237	-221
-13	169	195
-12	-82	-80
-11	-82	-62
-10	-82	70
-9	140	157
-8	-79	53
-7	227	-238
-6	166	156
-5	425	-440
-4	-81	4

L	FO	FC
-3	-80	49
-2	512	516
-1	582	562

H= 9, K= 13

L	FO	FC
0	264	-235
-15	289	270
-14	315	-295
-13	-84	0
-12	170	183
-11	-85	64
-10	149	139
-9	-83	-26
-8	434	-425
-7	278	-280
-6	193	187
-5	270	254
-4	240	256
-3	189	154
-2	-83	-23
-1	-83	73

H= 0, K= 14

L	FO	FC
0	746	-779
1	-81	-50
2	-80	-41
3	502	-479
4	-80	62
5	313	315
6	411	409
7	407	399
8	117	-125
9	281	-271
10	-81	-54
11	-82	65
12	146	120
13	157	112
14	191	-200
15	-84	46

H= 2, K= 14

L	FO	FC
0	128	-140
1	123	-164
2	465	463
3	-81	41
4	277	252
5	344	358
6	-80	-32
7	355	-335
8	132	-110
9	161	-134
10	199	182
11	-85	25
12	-87	-144
13	238	-205
-16	194	-182
-15	-82	4
-14	-84	-64
-13	204	-182
-12	170	220
-11	-81	106
-10	-81	-122
-9	-80	-104
-8	224	201
-7	462	-451
-6	165	183
-5	411	410
-4	201	-203
-3	130	104
-2	542	-575
-1	178	-189

H= 4, K= 14

L	FO	FC
0	565	555
1	-83	-112
2	133	133
3	475	438
4	-83	4
5	117	-59
6	357	-369
7	313	-298
8	-85	83
9	225	214
10	142	113
-17	213	-162
-15	211	-209
-15	-84	-86
-14	186	205
-13	-83	86
-12	126	-73
-11	210	220
-10	142	80
-9	148	-150
-8	270	281
-7	251	270
-6	314	-346
-5	208	240
-4	-81	-47
-3	328	-320
-2	-81	-116
-1	-79	-16

H= 6, K= 14

L	FO	FC
0	339	332
1	275	233
2	361	-378
3	-83	-6
4	283	-271
5	365	-355
6	-86	30
-16	128	114
-15	-86	-67
-14	-84	92
-13	234	225
-12	164	-179
-11	-82	-41
-10	-84	51
-9	-83	34
-8	188	-163
-7	447	418
-6	181	-151
-5	300	-324
-4	-81	58
-3	320	-294
-2	422	442
-1	-83	50

H= 8, K= 14

L	FO	FC
0	382	-377
-13	-84	-53
-12	-83	-36
-11	-85	-115
-10	-84	-29
-9	202	202
-8	313	-325
-7	140	-157
-6	204	216
-5	263	-270
-4	130	146
-3	239	224
-2	206	210
-1	-84	62

H= 1, K= 15

L	FO	FC
0	422	-428
1	455	-429
2	135	115
3	421	404
4	491	460
5	-82	97
6	147	-119
7	198	-165
8	280	-242
9	-85	-114
10	-84	55
11	245	221
-13	440	-445
-12	130	-47
-11	379	377
-10	-82	-6
-9	265	279
-8	191	153
-7	199	-158
-6	433	436
-5	402	-438
-4	-83	93
-3	300	294
-2	371	-402
-1	-82	15

H= 3, K= 15

L	FO	FC
0	302	310
1	-83	-38
2	360	346
3	258	288
4	-85	86
5	249	-257
6	326	-307
7	127	-100
8	260	-185
-13	207	202
-12	196	149
-11	427	398
-10	-85	30
-9	-82	-18
-8	298	310
-7	229	-210
-6	-84	57
-5	-85	-23
-4	537	-525
-3	346	347
-2	173	-120
-1	339	-321

H= 5, K= 15

L	FO	FC
0	501	496
1	353	345
2	-86	38
3	242	-250
4	361	-362
-13	466	474
-12	191	147
-11	152	-167
-10	-84	11
-9	237	-253
-8	161	-146
-7	-84	36
-6	379	-389
-5	372	377
-4	263	-245
-3	230	-209
-2	178	184
-1	172	-132

H= 7, K= 15

L	FO	FC
-8	274	-287
-7	230	229
-6	170	-171
-5	-86	28
-4	390	386
-3	328	-334

H= 0, K= 16

L	FO	FC
0	237	-274
1	-85	-93
2	153	113
3	140	91
4	-84	79
5	273	253
6	-84	-38
7	199	-163
8	132	146

H= 2, K= 16

L	FO	FC
0	-85	46
1	-84	-77
2	-85	123
3	-85	133
4	185	132
5	-86	-72
-9	351	354
-8	157	155
-7	404	-410
-6	285	-242
-5	174	-191
-4	241	-255
-3	167	196
-2	146	-125
-1	-85	17

H= 4, K= 16

L	FO	FC
0	264	249
1	-86	109
-7	253	-249
-6	-85	-53
-5	230	217
-4	-86	-103
-3	129	134
-2	140	-122

Table B-5

Observed and Calculated Structure Factors for $C_4(fph)_4Rh(cp)(tpp)$

L	FO	FC
H=	0, K=	0
1	-21	1092
2	1897	-1630
3	871	-822
4	213	-104
5	908	856
6	334	-311
7	1247	-1240
8	631	-596
9	719	733
10	361	344
11	-50	39
12	392	-395
13	144	-172
14	539	536
15	214	234
16	325	-322
17	138	-173
H=	0, K=	1
0	1644	-2458
1	155	-81
2	301	-154
3	1179	1084
4	332	-259
5	1289	-1263
6	128	-108
7	537	519
8	389	423
9	254	-248
10	410	-423
11	-63	-6
12	427	403
13	120	134
14	282	-283
15	-66	1
16	225	237
-18	-67	-9
-17	158	174
-16	192	187
-15	-69	-90
-14	383	-375
-13	-53	-52
-12	432	435
-11	128	134
-10	820	-842
-9	331	-304
-8	257	250
-7	631	607
-6	308	235
-5	999	-915
-4	102	-36
-3	508	553
-2	1102	1449
-1	552	-650
H=	0, K=	2
0	797	195
1	444	-363
2	611	-772
3	1243	-1280
4	157	223
5	1147	1107
6	77	14
7	348	-375
8	368	-344
9	243	252
10	329	334
11	-66	-30
12	323	-317
13	-67	36
14	301	301
15	-70	38
-19	104	88
-18	177	173
-17	-65	22
-16	190	-191
-15	187	183
-14	172	157
-13	-61	-60
-12	617	-621
-11	541	-504
-10	465	453
-9	313	299
-8	522	-537
-7	1485	-1493
-6	-54	-53
-5	1687	1629
-4	353	429
-3	-45	189
-2	920	-548
-1	106	154
H=	0, K=	3
0	1047	699
1	307	-260
2	589	525
3	464	442
4	149	186
5	274	218
6	-55	-12
7	257	279
8	-62	104
9	211	-197
10	330	-338
11	-69	85
12	293	296
13	-69	-64
14	130	-128
-19	244	-243
-18	311	-310
-17	357	368
-16	-66	94
-15	239	-232
-14	158	-146
-13	116	-89
-12	140	145
-11	382	406
-10	-54	-154
-9	196	-201
-8	220	201
-7	359	322
-6	163	-210
-5	964	-1036
-4	254	-223
-3	949	-776
-2	116	253
-1	1145	-997
H=	0, K=	4
0	-57	-64
1	286	307
2	591	-610
3	624	-619
4	324	328
5	628	605
6	122	-103
7	456	-488
8	141	-112
9	-66	60
10	165	153
11	260	-261
12	358	-352
13	104	-125
-20	150	-138
-19	390	384
-18	-66	2
-17	414	-407
-16	-64	-18
-15	-63	71
-14	323	336
-13	374	348
-12	410	-402
-11	496	-515
-10	176	180
-9	409	431
-8	217	208
-7	238	-262
-6	180	-226
-5	1102	1068
-4	838	897
-3	550	-509
-2	682	-613
-1	-57	25
H=	0, K=	5
0	353	347
1	337	-371
2	648	646
3	993	986
4	201	-269
5	460	-475
6	167	165
7	235	223
8	165	151
9	143	-156
10	305	-305
11	135	164
12	238	252
-20	-68	56
-19	315	-307
-18	-65	-52
-17	423	428
-16	218	237
-15	184	175
-14	222	-226
-13	108	96
-12	862	852
-11	720	741
-10	94	122
-9	487	-477
-8	341	-323
-7	470	-464
-6	417	341
-5	662	-722
-4	1307	-1306
-3	1195	1156
-2	130	165
-1	418	475
H=	0, K=	6
0	1116	1108
1	385	379
2	188	-178
3	215	-210
4	169	189
5	355	357
6	145	129
7	213	-212
8	192	-205
9	132	147
10	-71	98
11	-72	-88
-20	-67	-66
-19	177	177
-18	139	147
-17	183	-191
-16	627	-638
-15	-65	-124
-14	279	283
-13	135	-146
-12	330	-344
-11	693	-680
-10	-52	61
-9	990	589
-8	209	211
-7	461	-489
-6	526	-544
-5	-56	45
-4	-56	-6
-3	567	-560
-2	90	6
-1	470	-415
H=	0, K=	7
0	590	-603
1	105	-107
2	406	415
3	-66	-8
4	-67	1
5	252	-241
6	173	-164
7	244	249
8	113	132
9	205	-188
-21	242	237
-20	-67	81
-19	98	-86
-18	-64	-71
-17	-65	-41
-16	452	449
-15	217	216
-14	395	-389
-13	180	-188
-12	300	309
-11	441	415
-10	145	-149
-9	438	-458
-8	378	-381
-7	176	199
-6	102	41
-5	330	-337
-4	-54	-20
-3	134	128
-2	326	367
-1	275	292
H=	0, K=	8
0	230	235
1	242	-241
2	-67	57
3	-70	-94
4	140	-118
5	262	269
6	-70	73
7	214	-245
8	108	-72
-21	326	-325
-20	-68	-103
-19	-57	60
-18	173	167
-17	-68	146
-16	401	-380
-15	-65	-7
-14	445	455
-13	247	232
-12	148	-176
-11	425	-414
-10	194	206
-9	464	474
-8	116	-88
-7	541	-546
-6	300	-295
-5	573	557
-4	390	392
-3	-60	-22
-2	799	-823
-1	145	-142
H=	0, K=	9
0	444	-449

L	FO	FC
1	380	-393
2	310	302
3	323	311
4	-68	12
5	112	-95
6	-70	-40
-20	108	115
-19	-66	79
-18	253	-260
-17	-66	63
-16	444	449
-15	181	-170
-14	522	-534
-13	-63	11
-12	-62	25
-11	-62	27
-10	168	-182
-9	228	-250
-8	-61	-24
-7	288	308
-6	203	221
-5	271	-265
-4	190	-230
-3	287	-277
-2	529	527
-1	-68	-65

H= 0, K= 10

0	430	426
1	110	144
2	-68	-99
3	112	-125
4	-71	-49
-20	174	-173
-19	-67	76
-18	290	286
-17	360	-377
-16	488	-493
-15	241	251
-14	575	566
-13	397	397
-12	174	-196
-11	228	-233
-10	343	345
-9	603	601
-8	-66	82
-7	378	-370
-6	-68	-136
-5	107	94
-4	421	400
-3	-70	110
-2	455	-481
-1	-71	-75

H= 0, K= 11

0	-70	-35
1	170	-149
2	-73	72
-20	179	168
-19	244	-254
-18	174	-190
-17	154	156
-16	180	-172
-15	166	165
-14	-65	-10
-13	309	-311
-12	350	363
-11	340	356
-10	172	-188
-9	225	-236
-8	161	-121
-7	152	143
-6	247	256
-5	155	-177
-4	385	-373
-3	-69	90

L	FO	FC
-2	-67	17
-1	-67	-80

H= 0, K= 12

0	117	108
-19	265	269
-18	260	270
-17	-56	-36
-16	254	-233
-15	-67	-63
-14	177	174
-13	233	252
-12	186	-220
-11	345	-351
-10	100	49
-9	283	270
-8	138	172
-7	243	-255
-6	169	-150
-5	-69	64
-4	129	159
-3	218	-229
-2	145	-139
-1	-71	-48

H= 0, K= 13

-17	125	108
-16	132	134
-15	100	92
-14	147	-138
-13	225	-231
-12	-66	34
-11	-70	122
-10	-67	67
-9	-69	-56
-8	109	-107
-7	-69	51
-6	107	136
-5	166	-146
-4	-73	-128
-3	106	120

H= 0, K= 14

-15	137	-122
-14	160	186
-13	208	206
-12	-72	-149
-11	216	-219
-10	-70	47
-9	171	165
-8	148	138
-7	-72	-74

H= 1, K= 0

0	833	871
1	1365	-1608
2	570	-441
3	284	-369
4	710	-636
5	927	899
6	1064	-1021
7	1457	-1491
8	177	148
9	228	216
10	-65	94
11	248	-267
12	408	-404
13	-68	102
14	482	496
15	-69	-6
16	145	-175
-18	-69	-39
-17	393	-380
-16	150	-173

L	FO	FC
-15	521	499
-14	267	297
-13	300	-287
-12	236	-244
-11	324	-303
-10	159	172
-9	-52	61
-8	803	-796
-7	546	-567
-6	721	732
-5	1003	914
-4	704	-717
-3	314	-593
-2	682	-550
-1	1574	2416

H= 1, K= 1

0	514	-454
1	139	-216
2	799	929
3	188	134
4	267	-355
5	825	-755
6	864	856
7	780	788
8	272	-293
9	501	-492
10	210	-214
11	153	132
12	403	401
13	-66	-30
14	264	-256
15	-69	-63
16	147	136
-19	-67	-30
-18	-66	23
-17	192	217
-16	386	388
-15	161	-174
-14	310	-307
-13	103	109
-12	373	373
-11	125	147
-10	-51	-23
-9	365	-370
-8	115	190
-7	424	419
-6	604	-556
-5	700	-731
-4	457	-471
-3	73	-414
-2	606	237
-1	576	102

H= 1, K= 2

0	1635	1538
1	155	108
2	669	-546
3	283	-342
4	775	804
5	214	269
6	241	-343
7	458	-481
8	-59	-100
9	283	286
10	232	220
11	177	-153
12	405	-403
13	137	147
14	203	225
15	133	95
-19	188	180
-18	243	237
-17	313	-315
-16	181	-179
-15	134	122

L	FO	FC
-14	129	111
-13	-58	-13
-12	808	-781
-11	423	-445
-10	483	511
-9	962	909
-8	484	-438
-7	430	-413
-6	525	-433
-5	1231	1223
-4	403	307
-3	1347	-1618
-2	1408	-1657
-1	-51	317

H= 1, K= 3

0	904	-878
1	308	303
2	771	757
3	463	421
4	119	107
5	508	-471
6	98	-86
7	315	339
8	-64	-12
9	313	-305
10	276	-268
11	223	196
12	320	317
13	180	-176
14	245	-236
-20	-69	56
-19	354	-346
-18	-66	-45
-17	329	328
-16	132	106
-15	120	130
-14	324	-325
-13	247	-230
-12	696	683
-11	595	567
-10	-51	-90
-9	471	-481
-8	111	107
-7	297	362
-6	191	206
-5	269	-242
-4	1099	-1125
-3	1222	1037
-2	1268	1104
-1	715	741

H= 1, K= 4

0	340	297
1	215	205
2	890	-840
3	343	-347
4	636	608
5	341	349
6	178	177
7	117	103
8	144	-189
9	291	317
10	321	324
11	385	-386
12	169	-191
-20	-68	9
-19	261	258
-18	-64	5
-17	142	-155
-16	235	-214
-15	135	-151
-14	889	869
-13	219	223
-12	995	-988
-11	262	253

L	FO	FC
-10	940	894
-9	275	261
-8	-54	-85
-7	505	-454
-6	255	-214
-5	952	1021
-4	748	755
-3	853	-787
-2	169	49
-1	771	-699

H= 1, K= 5

L	FO	FC
0	530	-518
1	156	-174
2	736	703
3	136	130
4	112	-116
5	-63	-35
6	-66	57
7	224	241
8	129	129
9	341	-334
10	152	-156
11	180	169
-21	246	238
-20	-69	42
-19	326	-328
-18	122	-159
-17	-65	64
-16	156	172
-15	-61	-17
-14	573	-562
-13	183	164
-12	469	470
-11	185	171
-10	747	-758
-9	666	-691
-8	415	-379
-7	337	-319
-6	424	-372
-5	1191	-1149
-4	643	-549
-3	411	400
-2	319	243
-1	396	361

H= 1, K= 6

L	FO	FC
0	422	430
1	438	433
2	204	-203
3	126	-100
4	134	151
5	-68	79
6	-68	-5
7	234	-217
8	119	-125
9	-71	87
10	-71	66
-21	261	-276
-20	-68	-97
-19	228	245
-18	118	98
-17	254	-238
-16	202	-211
-15	274	269
-14	434	436
-13	255	235
-12	161	-205
-11	289	-287
-10	572	567
-9	442	442
-8	217	174
-7	218	-208
-6	690	-652
-5	423	415
-4	109	131

L	FO	FC
-3	93	-102
-2	704	-730
-1	-55	34

H= 1, K= 7

L	FO	FC
0	552	-550
1	141	-146
2	-66	81
3	-68	102
4	-68	19
5	254	-255
6	-69	-14
7	237	224
8	-73	-1
-21	254	249
-20	-65	-67
-19	152	-143
-18	-64	2
-17	277	271
-16	432	441
-15	184	-195
-14	507	-516
-13	85	-83
-12	-57	67
-11	149	167
-10	-55	54
-9	797	-809
-8	89	57
-7	779	800
-6	97	41
-5	594	-604
-4	169	-166
-3	-58	87
-2	550	547
-1	-59	0

H= 1, K= 8

L	FO	FC
0	-66	14
1	254	268
2	-70	71
3	331	-335
4	102	47
5	185	212
6	-70	63
7	175	-163
-21	172	-185
-20	155	160
-19	308	330
-18	339	334
-17	353	-356
-16	399	-385
-15	194	201
-14	236	262
-13	254	239
-12	160	-144
-11	310	-315
-10	311	328
-9	758	770
-8	206	-186
-7	464	-511
-6	138	-116
-5	311	293
-4	236	240
-3	173	-177
-2	433	-436
-1	107	-98

H= 1, K= 9

L	FO	FC
0	490	-514
1	-69	30
2	302	302
3	193	208
4	-71	79
5	211	-195
-21	98	87

L	FO	FC
-20	-67	-17
-19	267	-279
-18	371	-388
-17	416	415
-16	307	299
-15	496	-501
-14	323	-320
-13	-65	-109
-12	142	136
-11	456	466
-10	111	-102
-9	460	-480
-8	346	351
-7	602	604
-6	-63	33
-5	-65	30
-4	355	-333
-3	451	448
-2	299	308
-1	304	-307

H= 1, K= 10

L	FO	FC
0	164	168
1	-70	102
2	127	-100
3	179	-200
-20	-67	-79
-19	135	141
-18	104	102
-17	396	-416
-16	189	-192
-15	173	169
-14	502	529
-13	320	337
-12	239	-265
-11	264	-259
-10	196	216
-9	224	228
-8	134	-100
-7	289	-282
-6	268	-277
-5	106	92
-4	186	177
-3	234	-242
-2	278	-258
-1	-71	-79

H= 1, K= 11

L	FO	FC
0	177	-156
1	-74	-103
-20	129	152
-19	207	-199
-18	-66	-96
-17	-67	-40
-16	122	144
-15	200	221
-14	317	-305
-13	-66	-97
-12	322	336
-11	183	230
-10	244	-266
-9	183	-141
-8	-69	-49
-7	205	199
-6	194	179
-5	271	-280
-4	250	-248
-3	-67	10
-2	153	144
-1	-69	58

H= 1, K= 12

L	FO	FC
-19	252	256
-18	127	163
-17	191	-173

L	FO	FC
-16	222	-227
-15	-65	-24
-14	216	211
-13	177	156
-12	258	-265
-11	210	-207
-10	-67	47
-9	139	149
-8	147	167
-7	138	-123
-6	292	-301
-5	208	209
-4	133	121
-3	-70	-15
-2	109	-142

H= 1, K= 13

L	FO	FC
-17	-68	72
-16	188	202
-15	-68	66
-14	258	-269
-13	177	-173
-12	202	207
-11	185	198
-10	-69	-13
-9	100	-89
-8	-70	-63
-7	246	237
-6	179	175
-5	183	-187

H= 1, K= 14

L	FO	FC
-13	-74	93
-12	247	-275
-11	-71	-71

H= 1, K= -14

L	FO	FC
5	-70	68
6	206	-194
7	-69	-49
8	217	211
9	187	185
10	-68	-15
11	188	-169
12	119	-133
13	219	208
14	130	134
15	205	-177

H= 1, K= -13

L	FO	FC
2	137	154
3	-67	-3
4	282	-274
5	-66	10
6	-66	91
7	-63	40
8	-65	-26
9	-66	-86
10	122	-114
11	-63	18
12	169	153
13	224	-213
14	135	-132
15	102	124
16	149	147
17	-68	22

H= 1, K= -12

L	FO	FC
0	110	93
1	-66	-53
2	315	-321
3	-66	21
4	359	361

L	FO	FC
5	107	94
6	388	-387
7	179	-155
8	215	228
9	347	335
10	-66	81
11	406	-390
12	155	-163
13	202	217
14	165	149
15	92	-61
16	-64	-42
17	-68	-40
18	309	296
19	-67	0
-1	177	192

H= 1, K= -11

L	FO	FC
0	193	-170
1	-63	-29
2	279	276
3	110	-95
4	358	-354
5	-66	-68
6	210	208
7	190	159
8	-64	25
9	256	-263
10	99	-37
11	553	535
12	222	231
13	187	-182
14	96	124
15	-66	-126
16	147	146
17	211	192
18	252	-260
19	-67	-13
-3	274	271
-2	-66	48
-1	-64	-24

H= 1, K= -10

L	FO	FC
0	380	370
1	362	-352
2	357	-362
3	-64	12
4	303	286
5	180	197
6	571	-578
7	593	-601
8	320	312
9	431	424
10	140	-105
11	693	-714
12	-65	-46
13	519	527
14	364	347
15	207	-194
16	589	-613
17	-63	-15
18	108	109
19	-66	16
20	177	-164
-6	110	104
-5	298	286
-4	-68	-72
-3	268	-289
-2	146	-155
-1	556	559

H= 1, K= -9

L	FO	FC
0	470	-453
1	-62	24
2	-60	54
3	-60	-63
4	221	-260
5	375	-349
6	-58	-7
7	346	343
8	215	-229
9	445	-455
10	224	207
11	305	297
12	200	209
13	-62	-4
14	197	-202
15	-66	18
16	397	402
17	-63	-37
18	119	-109
19	-66	-90
20	116	129
-7	240	238
-6	-70	-98
-5	174	-188
-4	217	204
-3	294	285
-2	-67	83
-1	139	-153

H= 1, K= -8

L	FO	FC
0	320	340
1	568	-572
2	208	-246
3	84	83
4	619	577
5	348	338
6	268	-276
7	479	-487
8	283	286
9	345	378
10	-58	-87
11	328	-330
12	172	-174
13	109	60
14	271	266
15	-64	-47
16	215	-227
17	-64	-106
18	130	118
19	148	160
20	190	-190
-9	138	106
-8	165	-182
-7	278	-275
-6	175	180
-5	258	275
-4	-66	-40
-3	-63	0
-2	391	-336
-1	103	151

H= 1, K= -7

L	FO	FC
0	146	-166
1	392	391
2	92	-66
3	140	130
4	626	542
5	637	-556
6	-53	-1
7	393	417
8	-53	37
9	95	37
10	-55	-47
11	-57	-90
12	127	141
13	105	-84
14	462	-445
15	183	176
16	120	130
17	95	51
18	114	-64
19	125	-104
20	-66	29
-10	174	-157
-9	203	-171
-8	190	163
-7	308	325
-6	310	-296
-5	117	-100
-4	125	-110
-3	421	398
-2	598	590
-1	186	-182

H= 1, K= -6

L	FO	FC
0	712	664
1	470	410
2	406	-390
3	428	-398
4	474	455
5	429	471
6	674	-680
7	275	-253
8	-50	36
9	305	295
10	210	211
11	385	-390
12	280	-296
13	105	108
14	357	358
15	236	-235
16	-66	-59
17	121	143
18	293	287
19	224	205
20	-68	-35
-12	203	-220
-11	127	-117
-10	211	207
-9	-64	24
-8	334	-318
-7	176	-153
-6	188	174
-5	405	414
-4	258	272
-3	287	-383
-2	426	-414
-1	592	617

H= 1, K= -5

L	FO	FC
0	845	-887
1	1124	-1087
2	1322	1200
3	209	-233
4	944	-939
5	377	-320
6	112	-79
7	-54	119
8	146	-161
9	834	-810
10	361	-350
11	851	870
12	582	574
13	158	-189
14	-61	31
15	211	195
16	354	355
17	-63	-5
18	326	-313
19	235	-233
-13	-69	43
-12	274	266
-11	-66	-19
-10	353	-361
-9	-67	-106
-8	-65	64
-7	-62	15
-6	377	-356
-5	652	-655
-4	80	-70
-3	348	375
-2	364	363
-1	145	146

H= 1, K= -4

L	FO	FC
0	1574	1465
1	490	425
2	743	-923
3	244	-312
4	1010	1004
5	-54	92
6	1126	-1002
7	407	-409
8	246	-182
9	131	124
10	691	685
11	358	-374
12	446	-452
13	321	328
14	191	185
15	-64	-42
16	407	-422
17	182	-203
18	206	238
19	170	175
-14	-68	62
-13	-65	33
-12	434	-447
-11	133	-141
-10	415	412
-9	-62	-31
-8	360	-376
-7	-56	37
-6	-54	74
-5	806	797
-4	316	303
-3	821	-795
-2	422	-443
-1	981	1123

H= 1, K= -3

L	FO	FC
0	2217	-1990
1	654	563
2	1744	1547
3	283	163
4	820	-778
5	267	-253
6	156	-123
7	265	250
8	-53	-30
9	556	-558
10	294	-276
11	352	354
12	386	390
13	170	-208
14	268	-280
15	271	-299
16	325	324
17	-66	53
18	248	-256
-15	-69	-5
-14	239	-237
-13	-64	34
-12	355	355
-11	-63	-47
-10	218	-230
-9	115	-106
-8	254	244
-7	553	555
-6	361	390
-5	538	-532

L	FO	FC
-4	-54	-77
-3	599	685
-2	479	-602
-1	1237	-870

H= 1, K= -2

L	FO	FC
0	923	1091
1	502	234
2	689	-822
3	292	-284
4	793	823
5	858	751
6	599	-540
7	745	-693
8	190	151
9	586	568
10	201	207
11	699	-701
12	297	-259
13	146	-132
14	202	209
15	254	248
16	-66	-1
17	-68	-49
18	-71	120
-16	165	-135
-15	134	166
-14	231	258
-13	-65	7
-12	131	-114
-11	-62	92
-10	581	564
-9	168	180
-8	475	-479
-7	914	-939
-6	119	129
-5	1432	1308
-4	201	-264
-3	1120	-1131
-2	1063	841
-1	142	729

H= 1, K= -1

L	FO	FC
0	794	-778
1	1464	1145
2	1122	986
3	87	-176
4	911	811
5	970	-904
6	1006	974
7	1558	1455
8	76	65
9	540	-560
10	-56	-51
11	360	378
12	200	223
13	118	-102
14	460	-458
15	-69	39
16	248	239
17	143	166
-17	275	264
-16	159	163
-15	274	-255
-14	117	-125
-13	221	214
-12	-60	22
-11	162	-170
-10	283	-278
-9	340	-358
-8	121	-93
-7	319	257
-6	842	-756
-5	430	-541
-4	103	127
-3	1042	799
-2	199	-83
-1	137	951

H= 2, K= 0

L	FO	FC
0	1073	1159
1	146	-291
2	371	-360
3	694	555
4	132	-145
5	261	247
6	862	-632
7	599	-573
8	286	289
9	195	184
10	-63	89
11	286	-273
12	269	-268
13	561	581
14	287	314
15	-68	-85
-19	-59	56
-18	-67	29
-17	193	-204
-16	-65	9
-15	630	619
-14	294	280
-13	-61	25
-12	212	-192
-11	85	75
-10	883	911
-9	883	847
-8	938	-943
-7	562	-589
-6	310	319.
-5	875	-766
-4	104	135
-3	1320	-814
-2	212	-558
-1	1120	909

H= 2, K= 1

L	FO	FC
0	89	126
1	1190	989
2	-55	27
3	427	-302
4	734	-781
5	363	-408
6	1024	1029
7	203	236
8	407	-412
9	276	-267
10	153	-134
11	262	281
12	191	184
13	309	-306
14	129	-189
-19	190	-159
-18	194	-171
-17	437	440
-16	167	176
-15	377	-370
-14	254	-255
-13	-59	-85
-12	386	375
-11	-63	77
-10	555	-558
-9	358	-364
-8	452	431
-7	609	-640
-6	132	93
-5	931	-847
-4	2124	-1952
-3	251	595
-2	1197	834
-1	1746	1556

H= 2, K= 2

L	FO	FC
0	145	-68
1	310	196
2	295	-212
3	241	-245
4	332	306
5	607	593
6	242	-291
7	254	-230
8	344	341
9	348	338
10	231	234
11	259	-264
12	122	-107
13	-69	123
14	-73	124
-20	-68	63
-19	412	403
-18	130	138
-17	446	-455
-16	-64	-16
-15	220	200
-14	377	381
-13	-57	-38
-12	281	-295
-11	92	-66
-10	426	452
-9	-55	25
-8	162	116
-7	472	-493
-6	765	601
-5	1305	1291
-4	374	451
-3	102	132
-2	701	569
-1	94	120

H= 2, K= 3

L	FO	FC
0	708	-661
1	-55	-26
2	445	496
3	440	424
4	179	-226
5	-53	-85
6	362	375
7	173	156
8	105	-134
9	363	-358
10	217	-245
11	292	301
12	-68	42
-20	103	-110
-19	490	-480
-18	107	-99
-17	306	311
-16	-63	64
-15	229	-219
-14	535	-505
-13	224	-210
-12	285	307
-11	252	272
-10	223	-189
-9	350	-390
-8	80	72
-7	841	788
-6	-54	-102
-5	684	-749
-4	268	248
-3	510	624
-2	397	-409
-1	1343	-1248

H= 2, K= 4

L	FO	FC
0	416	405
1	79	-80
2	755	-736
3	130	137
4	421	408
5	298	290
6	285	280
7	316	-319
8	-67	-4
9	496	480
10	-68	-48
11	160	-173
-21	243	-231
-20	156	164
-19	418	414
-18	-64	-13
-17	218	-206
-16	118	-153
-15	211	181
-14	595	585
-13	313	-318
-12	318	-348
-11	148	165
-10	73	-16
-9	588	603
-8	-54	-78
-7	1205	-1232
-6	363	317
-5	691	600
-4	1053	-1066
-3	1311	-1220
-2	1236	-1175
-1	-57	13

H= 2, K= 5

L	FO	FC
0	171	-173
1	-57	2
2	724	720
3	288	301
4	294	-312
5	257	-257
6	-68	-79
7	280	269
8	118	15
9	309	-316
10	-72	-84
-21	198	196
-20	188	-186
-19	448	-456
-18	-63	2
-17	151	111
-16	243	270
-15	-60	-15
-14	293	-301
-13	-57	87
-12	785	801
-11	-53	19
-10	315	-308
-9	191	-196
-8	179	198
-7	407	431
-6	108	-143
-5	1211	-1229
-4	-58	-125
-3	1007	1030
-2	520	516
-1	77	80

H= 2, K= 6

L	FO	FC
0	617	600
1	164	177
2	492	-503
3	94	-108
4	-68	60
5	287	284
6	-68	71
7	298	-303
8	-71	-128

L	FO	FC
9	193	198
-21	195	-198
-20	103	85
-19	150	180
-18	150	141
-17	172	-194
-16	352	-353
-15	268	284
-14	594	617
-13	129	114
-12	435	-437
-11	192	218
-10	223	245
-9	555	564
-8	231	-243
-7	987	-984
-6	261	-235
-5	136	87
-4	581	576
-3	153	-141
-2	416	-430
-1	249	-254

H= 2, K= 7

L	FO	FC
0	544	-535
1	-68	-50
2	165	182
3	121	107
4	152	-142
5	189	-189
6	-71	89
7	265	259
-21	140	125
-20	-66	-31
-19	-64	93
-18	-66	-85
-17	293	301
-16	339	362
-15	349	-366
-14	445	-470
-13	-60	31
-12	440	439
-11	230	236
-10	406	-421
-9	222	-202
-8	889	871
-7	305	336
-6	138	-146
-5	-57	-31
-4	344	-323
-3	297	286
-2	441	473
-1	-64	37

H= 2, K= 8

L	FO	FC
0	207	218
1	123	96
2	128	-138
3	99	-34
4	154	139
5	250	239
-21	-67	-63
-20	148	91
-19	-65	27
-18	-64	48
-17	477	-463
-16	237	-242
-15	-65	41
-14	154	160
-13	100	130
-12	306	-315
-11	341	-348
-10	453	447
-9	131	174
-8	229	-222
-7	343	-328
-6	361	-348
-5	108	127
-4	582	590
-3	334	-362
-2	463	-462
-1	135	130

H= 2, K= 9

L	FO	FC
0	278	-272
1	-69	37
2	131	108
3	104	113
4	188	-167
-21	-66	-38
-20	106	-94
-19	189	-184
-18	-64	-56
-17	528	518
-16	128	-101
-15	394	-351
-14	-66	-74
-13	-65	17
-12	324	330
-11	195	200
-10	475	-492
-9	132	-152
-8	444	445
-7	332	322
-6	312	308
-5	416	-421
-4	104	-31
-3	390	385
-2	144	-152
-1	453	-459

H= 2, K= 10

L	FO	FC
0	202	191
1	-71	53
2	120	-123
-21	-68	-30
-20	-67	-59
-19	267	267
-18	192	177
-17	292	-295
-16	102	-101
-15	228	252
-14	362	377
-13	99	58
-12	272	-261
-11	245	-241
-10	257	262
-9	265	251
-8	183	-153
-7	266	-270
-6	120	-100
-5	225	226
-4	106	96
-3	-69	-60
-2	374	-368
-1	-69	1

H= 2, K= 11

L	FO	FC
-20	-69	-5
-19	393	-393
-18	130	-144
-17	-65	40
-16	165	117
-15	99	-103
-14	237	-242
-13	-66	-23
-12	449	472
-11	-66	30
-10	173	-214
-9	-68	26
-8	134	144
-7	201	218
-6	-68	-42
-5	432	-442
-4	152	-103
-3	220	208
-2	104	125
-1	-71	-6

H= 2, K= 12

L	FO	FC
-18	123	67
-17	-68	-93
-16	129	-109
-15	-66	42
-14	229	228
-13	-69	103
-12	204	-191
-11	141	-163
-10	-65	15
-9	185	197
-8	-69	85
-7	253	-262
-6	-72	81
-5	302	313
-4	-72	93

H= 2, K= 13

L	FO	FC
-16	143	156
-15	122	-66
-14	151	-168
-13	-69	44
-12	163	186
-11	-71	22
-10	-70	-64
-9	-72	-94
-8	-72	-6

H= 2, K= -14

L	FO	FC
4	259	237
5	-70	-50
6	220	-203
7	-67	5
8	198	194
9	225	220
10	-69	-45
11	347	-338
12	-67	-103
13	258	251
14	-67	-2
15	193	-166

H= 2, K= -13

L	FO	FC
0	-68	-25
1	111	98
2	162	165
3	143	-128
4	195	-196
5	-66	-29
6	139	146
7	147	162
8	123	-113
9	169	-201
10	-64	-36
11	311	305
12	-65	-2
13	160	-168
14	-65	64
15	-70	129
16	147	157
17	-67	16

H= 2, K= -12

L	FO	FC
0	133	152
1	156	-171
2	207	-203
3	265	259
4	300	298
5	210	-198
6	382	-385
7	98	-71
8	200	210
9	259	260
10	247	-253
11	275	-285
12	-65	-20
13	115	105
14	123	128
15	154	156
16	194	-195
17	-66	73
18	238	234
-2	112	101
-1	131	138

H= 2, K= -11

L	FO	FC
0	-66	-55
1	111	64
2	-66	-10
3	277	-275
4	443	-464
5	120	-58
6	195	177
7	164	160
8	-64	73
9	163	-172
10	111	67
11	484	473
12	59	-67
13	348	-353
14	-67	-112
15	-65	-3
16	225	242
17	155	-175
18	301	-294
19	-68	25
-4	302	293
-3	249	256
-2	105	99
-1	-67	0

H= 2, K= -10

L	FO	FC
0	148	155
1	414	-434
2	307	-299
3	229	240
4	373	383
5	113	-114
6	483	-499
7	310	-309
8	94	-110
9	255	289
10	260	-262
11	245	-248
12	215	212
13	424	427
14	304	295
15	393	-355
16	239	-253
17	136	119
18	309	306
19	-67	-30
-6	396	386
-5	202	213
-4	293	-289
-3	137	-161
-2	218	217
-1	404	403

H= 2, K= -9

L	FO	FC
0	737	-732
1	160	144
2	265	277
3	124	112
4	295	-294
5	110	-139
6	513	506
7	427	445
8	306	-341
9	-59	-74
10	-60	14
11	91	60
12	394	387
13	-64	-77
14	401	-398
15	294	319
16	184	166
17	194	-210
18	328	-325
19	-65	24
-8	267	280
-7	136	114
-6	141	-178
-5	99	-120
-4	-65	15
-3	120	161
-2	314	333
-1	496	-495

H= 2, K= -8

L	FO	FC
0	649	644
1	-56	-26
2	431	-429
3	315	312
4	662	637
5	191	195
6	703	-710
7	277	-288
8	698	701
9	305	312
10	111	88
11	329	-331
12	344	-338
13	278	293
14	260	254
15	237	-232
16	138	-122
17	-63	40
18	220	238
19	115	83
-10	185	210
-9	-68	5
-8	273	-283
-7	354	-337
-6	325	338
-5	283	289
-4	-64	40
-3	345	-328
-2	272	-296
-1	748	773

H= 2, K= -7

L	FO	FC
0	393	-356
1	201	164
2	376	423
3	860	830
4	159	-178
5	583	-622
6	717	746
7	227	213
8	893	-889
9	539	-512
10	617	-598
11	385	366
12	410	411
13	526	-548
14	-63	4
15	206	207
16	274	268
17	-65	100
18	96	-83
19	212	-220
-11	-69	19
-10	257	-247
-9	191	-205
-8	359	363
-7	-65	9
-6	251	-236
-5	271	-278
-4	253	-244
-3	458	447
-2	161	163
-1	709	-700

H= 2, K= -6

L	FO	FC
0	104	24
1	1029	-1015
2	881	-770
3	100	-54
4	122	-124
5	96	-131
6	555	-570
7	886	-874
8	135	177
9	761	720
10	-54	15
11	447	-438
12	231	-279
13	260	258
14	118	104
15	151	154
16	304	-295
17	-64	39
18	196	204
19	206	178
-13	139	-108
-12	205	-200
-11	-55	10
-10	171	176
-9	-66	-65
-8	399	-386
-7	255	-242
-6	146	170
-5	523	524
-4	172	-178
-3	333	-363
-2	408	442
-1	811	786

H= 2, K= -5

L	FO	FC
0	649	610
1	1472	1453
2	384	441
3	258	-219
4	528	-587
5	741	-754
6	438	369
7	510	473
8	175	-129
9	238	-334
10	251	255
11	664	674
12	127	117
13	126	-87
14	-65	-117
15	107	-127
16	148	147
17	-64	-61
18	257	-232
19	133	-154
-14	-69	-102
-13	-69	107
-12	231	236
-11	-65	-61
-10	286	-270
-9	-63	-64
-8	123	116
-7	-58	-2
-6	247	-231
-5	930	-910
-4	186	168
-3	703	735
-2	91	-154
-1	322	322

H= 2, K= -4

L	FO	FC
0	96	127
1	348	-216
2	947	-838
3	225	-215
4	753	726
5	135	114
6	298	-294
7	536	-536
8	689	-646
9	565	590
10	126	103
11	543	-548
12	-59	-47
13	-61	-16
14	-63	16
15	-66	-99
16	-66	-87
17	-66	-40
18	276	284
-15	-69	92
-14	259	276
-13	166	-171
-12	308	-319
-11	147	118
-10	195	207
-9	99	-96
-8	197	176
-7	317	-345
-6	260	287
-5	1337	1306
-4	136	128
-3	229	-232
-2	294	193
-1	112	-215

H= 2, K= -3

L	FO	FC
0	846	-753
1	201	-58
2	1288	1335
3	-54	3
4	172	-181
5	492	480
6	496	495
7	940	925
8	449	-438
9	603	-621
10	202	188
11	532	529
12	-62	-104
13	95	86
14	239	-236
15	-66	32
16	231	236
17	-66	-9
18	209	-220
-16	163	175
-15	140	-160
-14	247	-256
-13	158	174
-12	241	219
-11	-62	36
-10	425	-403
-9	-57	-78
-8	100	115
-7	404	403
-6	-56	-13
-5	283	-249
-4	-52	15
-3	120	13
-2	1162	894
-1	344	78

H= 2, K= -2

L	FO	FC
0	966	1066
1	1474	1446
2	1016	-976
3	1064	1036
4	322	315
5	118	-96
6	99	-101
7	677	-654
8	394	404
9	428	405
10	112	-150
11	200	-198
12	285	-298
13	191	178
14	618	624
15	-67	10
16	254	-261
17	-69	-16
-17	208	-218
-16	230	-231
-15	130	124
-14	201	198
-13	94	-113
-12	448	-456
-11	158	128
-10	528	521
-9	240	-212
-8	453	-434
-7	614	-624
-6	404	443
-5	-53	94
-4	518	-511
-3	1459	-1084
-2	1356	-1697
-1	195	-540

H= 2, K= -1

L	FO	FC
0	773	-489
1	618	625
2	525	528
3	695	-622
4	428	-459
5	234	232
6	649	597
7	107	145
8	646	-658
9	202	-196
10	306	-289
11	237	236
12	271	259
13	893	-940
14	408	-411
15	183	177
16	299	295
-18	-67	28
-17	179	161
-16	-67	113
-15	143	-154
-14	96	-56
-13	-62	38
-12	370	350
-11	-56	-16

L	FO	FC
-10	748	-736
-9	688	-709
-8	519	482
-7	367	335
-6	108	-64
-5	978	-893
-4	257	316
-3	1128	1530
-2	453	-25
-1	880	-1233

H= 3, K= 0

L	FO	FC
0	131	-6
1	344	-294
2	-54	-3
3	100	-71
4	210	266
5	631	627
6	544	-554
7	-56	-90
8	380	366
9	-63	60
10	196	202
11	293	-310
12	-66	-18
13	239	239
14	133	148
-19	252	254
-18	-67	56
-17	357	-360
-16	262	263
-15	507	493
-14	-63	51
-13	-60	104
-12	286	-295
-11	168	-201
-10	670	720
-9	402	-367
-8	962	-926
-7	385	-336
-6	776	-715
-5	171	-179
-4	1654	1190
-3	1724	-1491
-2	115	48
-1	1633	1429

H= 3, K= 1

L	FO	FC
0	496	484
1	728	635
2	622	627
3	-56	-2
4	620	-570
5	-56	92
6	313	303
7	-59	7
8	132	-123
9	221	-215
10	157	-172
11	458	459
12	213	208
13	131	-135
-20	158	-155
-19	351	-336
-18	-65	-19
-17	314	307
-16	-65	-11
-15	294	-274
-14	421	-425
-13	-56	-29
-12	455	461
-11	190	-211
-10	891	-892
-9	539	531
-8	559	562
-7	892	889
-6	384	-305
-5	1429	-1334
-4	937	599
-3	903	970
-2	133	128
-1	172	-262

H= 3, K= 2

L	FO	FC
0	478	509
1	227	-235
2	1216	-1233
3	450	-401
4	849	682
5	207	203
6	255	-264
7	126	-97
8	-63	4
9	414	402
10	105	113
11	369	-366
12	209	-226
-20	-71	129
-19	324	303
-18	127	-106
-17	292	-273
-16	141	-138
-15	159	154
-14	249	234
-13	94	-86
-12	1065	-1055
-11	-53	11
-10	801	771
-9	92	106
-8	644	-654
-7	841	-711
-6	479	463
-5	138	210
-4	158	6
-3	941	-854
-2	942	-935
-1	218	-245

H= 3, K= 3

L	FO	FC
0	533	-505
1	564	527
2	634	629
3	-56	-35
4	575	-557
5	107	-70
6	138	154
7	256	243
8	-68	-67
9	451	-461
10	-69	96
11	194	180
-21	206	184
-20	117	-162
-19	233	-227
-18	184	178
-17	299	289
-16	-62	36
-15	267	-251
-14	319	-304
-13	246	267
-12	1075	1027
-11	195	183
-10	-51	54
-9	252	235
-8	794	757
-7	95	133
-6	477	-412
-5	577	-479
-4	765	-796
-3	412	-409
-2	398	377
-1	595	-602

H= 3, K= 4

L	FO	FC
0	370	399
1	-56	-43
2	399	-393
3	368	379
4	516	515
5	188	203
6	101	-89
7	293	-286
8	159	175
9	264	248
10	130	-50
-21	110	-178
-20	250	236
-19	-66	93
-18	141	-141
-17	125	-130
-16	182	-174
-15	273	290
-14	364	377
-13	361	-354
-12	428	-415
-11	226	223
-10	-52	30
-9	281	271
-8	370	-397
-7	481	-531
-6	-56	145
-5	73	125
-4	264	264
-3	323	-372
-2	241	-230
-1	329	341

H= 3, K= 5

L	FO	FC
0	515	-485
1	136	117
2	379	352
3	403	-422
4	199	-198
5	143	-144
6	115	136
7	412	417
8	-70	-84
9	226	-228
-21	152	140
-20	307	-314
-19	177	-169
-18	103	-78
-17	240	246
-16	318	306
-15	219	-220
-14	210	-219
-13	637	639
-12	407	427
-11	145	-157
-10	125	-133
-9	361	-394
-8	326	323
-7	1011	1021
-6	562	-571
-5	567	-515
-4	610	634
-3	527	530
-2	97	130
-1	305	-298

H= 3, K= 6

L	FO	FC
0	341	351
1	190	-204
2	191	-215
3	134	98
4	290	272
5	260	290
6	118	-157
7	332	-330
-21	120	-173
-20	100	98
-19	288	285
-18	-64	81
-17	452	-452
-16	154	-131
-15	408	420
-14	268	276
-13	173	-166
-12	142	-153
-11	158	-158
-10	668	691
-9	520	502
-8	727	-766
-7	807	-811
-6	212	226
-5	570	596
-4	194	[illegible]
-3	571	[illegible]
-2	288	-299
-1	370	357

H= 3, K= 7

L	FO	FC
0	397	-380
1	-69	22
2	225	211
3	-71	116
4	196	-191
5	213	-215
6	203	194
-21	-68	110
-20	110	-114
-19	192	-194
-18	104	-116
-17	357	344
-16	129	116
-15	590	-607
-14	224	-222
-13	100	84
-12	-59	19
-11	-60	-75
-10	565	-559
-9	129	155
-8	511	513
-7	156	173
-6	420	-414
-5	575	-580
-4	209	-195
-3	327	309
-2	320	325
-1	457	-442

H= 3, K= 8

L	FO	FC
0	100	119
1	-70	64
2	232	-210
3	179	-189
4	228	226
-21	-67	-69
-20	-65	44
-19	230	232
-18	110	113
-17	242	-252
-16	99	-104
-15	119	106
-14	-65	-1
-13	228	223
-12	413	-392
-11	-63	11
-10	425	427
-9	96	92
-8	-64	-63
-7	159	-163
-6	-66	15

L	FO	FC
-5	562	573
-4	-68	52
-3	503	-511
-2	128	125
-1	-70	100
H=	3, K=	9
0	264	-235
1	-70	0
2	143	178
-21	-67	63
-20	111	133
-19	-66	-73
-18	-65	-35
-17	160	157
-16	245	-258
-15	150	-150
-14	247	235
-13	-65	24
-12	343	339
-11	-67	2
-10	194	-206
-9	175	162
-8	232	233
-7	-68	86
-6	-68	-69
-5	-70	-138
-4	133	145
-3	-69	74
-2	-70	-66
-1	283	-276
H=	3, K=	10
0	113	125
-20	101	-78
-19	204	210
-18	-68	91
-17	166	-177
-16	116	-107
-15	-65	-13
-14	-66	36
-13	108	80
-12	348	-352
-11	-69	1
-10	263	251
-9	-68	32
-8	-67	-17
-7	115	-93
-6	-68	-40
-5	263	261
-4	217	223
-3	376	-379
-2	172	-175
-1	-74	125
H=	3, K=	11
-19	146	-153
-18	140	-126
-17	-69	45
-16	196	212
-15	126	112
-14	131	-144
-13	166	216
-12	260	250
-11	149	-128
-10	149	-143
-9	-66	-48
-8	116	106
-7	198	218
-6	-70	-92
-5	293	-280
-4	-71	42
-3	130	136
H=	3, K=	12

L	FO	FC
-18	137	97
-17	180	-198
-16	285	-283
-15	-69	43
-14	287	284
-13	-70	-46
-12	234	-235
-11	137	-146
-10	167	181
-9	165	176
-8	-72	-98
-7	213	-210
-6	104	65
H=	3, K=	-15
8	-70	-74
9	108	116
10	106	108
11	130	152
H=	3, K=	-14
3	122	119
4	192	160
5	123	-99
6	180	-188
7	-66	-31
8	106	118
9	128	121
10	118	-132
11	263	-263
12	-69	93
13	220	216
14	-66	-52
15	143	-129
H=	3, K=	-13
0	117	-88
1	-69	99
2	123	124
3	271	-241
4	194	-196
5	-64	66
6	324	315
7	-64	26
8	216	-205
9	268	-272
10	136	140
11	141	142
12	122	-106
13	107	-128
14	-66	-16
15	306	295
16	161	159
-1	-70	-99
H=	3, K=	-12
0	164	177
1	190	-208
2	120	-104
3	262	254
4	168	150
5	167	-173
6	311	-312
7	94	-100
8	262	269
9	218	212
10	213	-200
11	292	-286
12	149	-131
13	251	244
14	295	318
15	152	-159
16	175	-160

L	FO	FC
17	159	140
-3	-69	-94
-2	108	127
-1	208	222
H=	3, K=	-11
0	112	-139
1	334	283
2	176	199
3	409	-410
4	171	-163
5	160	165
6	186	182
7	119	71
8	250	-232
9	315	-300
10	507	501
11	299	303
12	528	-536
13	115	-134
14	-64	4
15	122	123
16	96	50
17	-57	-97
18	281	-264
-5	-73	-54
-4	288	282
-3	101	111
-2	-67	-85
-1	-64	-17
H=	3, K=	-10
0	-66	-67
1	686	-709
2	-63	64
3	177	165
4	-61	64
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6	385	-382
7	385	-365
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9	217	183
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13	405	427
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18	203	204
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11	522	511
12	259	256
13	505	-523
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L	FO	FC
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-6	164	-161
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-10	132	119
-9	-69	-121
-8	430	-442
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6	910	908
7	357	-326
8	485	-504
9	479	-462
10	287	-293
11	364	353
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13	333	-323
14	-63	-35
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16	326	318
17	122	81
18	276	-270
-12	212	216
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-10	328	-333
-9	117	138
-8	342	346
-7	120	-127
-6	176	-168
-5	328	-331
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-3	497	522

L	FO	FC
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-1	580	-536
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3	271	315
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6	950	-873
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8	869	812
9	192	203
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11	352	-371
12	143	-148
13	308	290
14	396	404
15	314	-315
16	202	-211
17	-67	49
18	270	248
-13	-71	-109
-12	227	-225
-11	-68	77
-10	299	281
-9	145	-135
-8	376	-356
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3	568	-518
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9	647	-637
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12	-62	-83
13	393	-415
14	440	-447
15	287	283
16	227	247
17	-67	-70
18	302	-287
-14	167	-155
-13	231	278
-12	160	168
-11	256	-247
-10	355	-383
-9	155	-142
-8	173	180
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-6	409	-443
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14	309	287
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16	331	-322
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-16	-70	-55
-15	207	196
-14	-67	97
-13	308	-314
-12	154	-159
-11	276	257
-10	534	527
-9	260	247
-8	642	-630
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-5	516	496
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8	609	-630
9	352	-364
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11	-60	-77
12	206	203
13	210	-209
14	362	-358
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17	162	-147
-17	131	104
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-15	340	-341
-14	138	-147
-13	292	285
-12	106	111
-11	450	-466
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-9	138	-122
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9	193	171
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15	218	-236
16	194	-172
-17	259	-259
-16	-67	-66
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-13	165	-143
-12	-60	61
-11	426	416
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-9	232	237
-8	216	-206
-7	452	-411
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3	923	-801
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5	151	157
6	610	602
7	340	333
8	558	-566
9	216	-222
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11	113	114
12	489	-494
13	322	-310
14	143	166
15	245	251
-18	-68	4
-17	313	296
-16	-64	38
-15	181	-194
-14	-66	80
-13	312	304
-12	110	107
-11	135	90
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-7	402	428
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-3	303	62
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5	189	-178
6	312	-324
7	143	-173
8	96	133
9	318	331
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11	249	-271
12	119	-106
13	251	244
-19	163	168
-18	250	-255
-17	251	-258
-16	273	262
-15	173	185
-14	-61	39
-13	246	-247
-12	597	-540
-11	117	-116
-10	279	273
-9	540	-536
-8	744	-757
-7	883	-917
-6	632	-638
-5	1530	1623
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2	401	376
3	468	-485
4	660	-658
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6	292	289
7	104	115
8	125	-140
9	382	-366
10	-67	63
11	229	212
12	-69	-4
-20	134	-145
-19	267	-289
-18	179	182
-17	286	298
-16	117	-125
-15	314	-322
-14	119	111
-13	281	293
-12	243	292
-11	284	-270
-10	95	-82
-9	784	705
-8	207	234
-7	422	287
-6	776	-800
-5	1192	-1016
-4	430	394
-3	397	425
-2	340	-245
-1	819	-789
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0	344	346
1	576	-520
2	765	-761
3	90	68
4	361	366
5	117	104
6	192	-198
7	194	-190
8	160	178
9	325	345
10	-68	-89
11	245	-236
-21	126	-109
-20	264	251
-19	333	324

L	FO	FC
-18	-65	-90
-17	232	-210
-16	191	189
-15	428	429
-14	159	154
-13	377	-420
-12	441	-406
-11	865	849
-10	676	652
-9	-51	4
-8	559	-535
-7	524	-489
-6	833	694
-5	1307	1266
-4	635	-605
-3	629	-607
-2	298	333
-1	1040	994

H= 4, K= 3

L	FO	FC
0	162	155
1	-57	42
2	459	452
3	144	175
4	253	-262
5	-65	-21
6	312	304
7	276	279
8	171	-151
9	179	-185
10	-69	48
-21	151	133
-20	261	-254
-19	151	-133
-18	-65	79
-17	103	126
-16	202	-230
-15	420	-425
-14	-60	-20
-13	439	444
-12	412	430
-11	436	-400
-10	610	-612
-9	387	429
-8	647	636
-7	383	372
-6	873	-936
-5	905	-868
-4	149	129
-3	590	557
-2	370	-335
-1	809	-851

H= 4, K= 4

L	FO	FC
0	445	429
1	338	-335
2	290	-270
3	275	292
4	269	268
5	189	200
6	148	-142
7	287	-306
8	191	195
9	126	141
-21	-68	-29
-20	163	173
-19	97	-82
-18	-62	6
-17	231	-236
-16	148	-146
-15	490	483
-14	-60	26
-13	627	-656
-12	243	-246
-11	155	156
-10	465	488

L	FO	FC
-9	419	436
-8	404	-389
-7	101	-140
-6	1356	1284
-5	625	636
-4	101	-102
-3	353	-352
-2	515	-537
-1	114	119

H= 4, K= 5

L	FO	FC
0	384	-375
1	378	380
2	160	165
3	-68	-7
4	305	-317
5	161	-154
6	358	359
7	215	249
-21	-67	-61
-20	255	-242
-19	148	-144
-18	-65	64
-17	320	307
-16	-64	23
-15	275	-297
-14	93	41
-13	482	477
-12	276	270
-11	-57	25
-10	472	-476
-9	124	-128
-8	533	550
-7	-56	91
-6	687	-688
-5	324	-329
-4	354	-363
-3	187	192
-2	261	242
-1	486	-484

H= 4, K= 6

L	FO	FC
0	240	219
1	366	-364
2	223	-203
3	-67	68
4	253	267
5	-69	34
6	273	-253
-22	225	-223
-21	-68	-83
-20	188	190
-19	186	195
-18	139	-127
-17	227	-234
-16	212	-228
-15	225	229
-14	-63	34
-13	314	-304
-12	152	-167
-11	96	72
-10	553	553
-9	-59	76
-8	497	-463
-7	277	-288
-6	209	-230
-5	-61	-9
-4	91	-80
-3	277	-264
-2	-65	-100
-1	490	473

H= 4, K= 7

L	FO	FC
0	176	-177
1	-68	108
2	224	230
3	-70	-46
4	269	-271
-21	-67	69
-20	113	-87
-19	150	-142
-18	-65	-25
-17	337	389
-16	325	323
-15	214	-226
-14	-66	101
-13	-63	-39
-12	266	263
-11	-63	49
-10	513	-514
-9	-62	-7
-8	231	236
-7	-64	33
-6	-65	34
-5	-65	27
-4	208	228
-3	627	624
-2	-71	54
-1	456	-469

H= 4, K= 8

L	FO	FC
0	-69	57
1	129	-100
2	240	-275
-21	208	-184
-20	137	134
-19	236	239
-18	-66	34
-17	333	-333
-16	450	-439
-15	100	-60
-14	221	225
-13	-68	118
-12	374	-372
-11	146	162
-10	508	529
-9	103	74
-8	-67	-55
-7	-66	-43
-6	115	121
-5	268	277
-4	236	-257
-3	-69	-74
-2	-68	27
-1	-68	36

H= 4, K= 9

L	FO	FC
0	102	-79
-21	379	360
-20	-68	-19
-19	267	-244
-18	-66	65
-17	234	227
-16	-65	-33
-15	-68	-102
-14	154	-128
-13	116	-119
-12	295	298
-11	98	-80
-10	251	-257
-9	168	175
-8	-67	62
-7	330	321
-6	-69	16
-5	304	-313
-4	-68	-66
-3	227	219
-2	-70	-79
-1	257	-226

H= 4, K= 10

L	FO	FC
-20	103	109
-19	151	163
-18	-68	-78
-17	316	-347
-16	-66	-93
-15	234	241
-14	239	252
-13	-66	-59
-12	216	-216
-11	-66	9
-10	-67	95
-9	-67	63
-8	106	-129
-7	212	-225
-6	118	146
-5	370	393
-4	-70	-46
-3	230	-226
-2	-71	-14

H= 4, K= 11

L	FO	FC
-18	-68	0
-17	149	164
-16	-68	71
-15	193	-222
-14	191	-183
-13	165	170
-12	169	152
-11	-65	-40
-10	154	-175
-9	-69	-52
-8	142	136
-7	160	184
-6	-73	-125
-5	205	-207

H= 4, K= 12

L	FO	FC
-16	-69	-32
-15	258	207
-14	-73	117
-13	178	-145
-12	167	-200
-11	112	-25
-10	158	174

H= 4, K= -15

L	FO	FC
7	115	-100
8	152	-145
9	123	-126
10	139	125

H= 4, K= -14

L	FO	FC
2	-70	-104
3	176	198
4	173	165
5	146	-157
6	231	-233
7	103	-92
8	103	113
9	175	160
10	168	-163
11	171	-175
12	203	183
13	129	139
14	-68	-43

H= 4, K= -13

L	FO	FC
0	141	131
1	275	307
2	-66	-43
3	253	-244
4	-66	-22

L	FO	FC
5	151	167
6	-64	-1
7	-65	-45
8	107	-118
9	-66	93
10	221	214
11	-66	67
12	96	-102
13	161	-179
14	104	106
15	238	226
16	-68	-26
-1	-68	0
H=	4, K=	-12
0	103	92
1	212	-167
2	-66	-73
3	301	297
4	-66	63
5	-65	-64
6	161	-133
7	-66	-17
8	352	359
9	152	-151
10	366	-392
11	310	-308
12	108	149
13	315	320
14	-68	89
15	216	-198
16	116	-88
17	253	273
-4	108	-131
-3	-67	-12
-2	-66	53
-1	-68	74
H=	4, K=	-11
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1	215	215
2	154	-153
3	401	-403
4	-64	-17
5	95	18
6	203	190
7	-65	-74
8	362	-344
9	198	214
10	451	435
11	257	-254
12	192	-200
13	98	-83
14	-65	-26
15	242	223
16	206	200
17	281	-276
-6	212	-209
-5	-68	35
-4	-67	85
-3	-64	-3
-2	210	217
-1	136	151
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2	207	-211
3	150	159
4	166	133
5	100	-30
6	573	-566
7	-63	38
8	475	491
9	132	116
10	-63	26
11	157	-136
12	105	47
13	465	467
14	103	107
15	340	-353
16	135	-152
17	211	217
-8	231	-222
-7	116	-119
-6	-67	42
-5	140	162
-4	144	-114
-3	-64	-53
-2	122	82
-1	194	176
H=	4, K=	-9
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2	87	-65
3	208	-200
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5	246	230
6	501	511
7	550	-549
8	489	-459
9	203	-217
10	-64	89
11	262	265
12	102	-115
13	487	-516
14	163	-169
15	263	255
16	-65	21
17	-66	-75
-10	208	-209
-9	-68	12
-8	306	299
-7	159	165
-6	261	-249
-5	-67	-60
-4	283	289
-3	323	323
-2	147	-121
-1	405	-409
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1	473	-434
2	150	-158
3	599	576
4	807	750
5	297	-303
6	638	-589
7	117	-84
8	402	412
9	406	379
10	261	-267
11	424	-442
12	381	383
13	438	440
14	-64	55
15	321	-323
16	281	-285
17	-67	47
-11	196	204
-10	229	239
-9	-66	-69
-8	170	-169
-7	209	197
-6	126	151
-5	147	162
-4	209	-224
-3	542	-525
-2	98	134
-1	500	498
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1	545	570
2	445	424
3	89	23
4	645	-657
5	339	287
6	463	458
7	-54	46
8	477	-490
9	529	-514
10	-60	87
11	426	402
12	334	-347
13	438	-440
14	242	261
15	421	445
16	239	239
17	-67	-3
-12	114	156
-11	191	-172
-10	153	-171
-9	292	298
-8	-65	29
-7	207	-199
-6	302	-306
-5	372	-378
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-2	848	-793
-1	349	-364
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1	358	-314
2	296	-299
3	540	532
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6	133	-139
7	263	-242
8	402	385
9	348	365
10	261	-247
11	391	-365
12	235	233
13	344	345
14	223	-248
15	249	-252
16	202	-194
17	-68	55
-14	-69	62
-13	188	-202
-12	-68	-40
-11	277	284
-10	118	-69
-9	409	-421
-8	431	-438
-7	162	-122
-6	180	189
-5	330	361
-4	374	-401
-3	160	-204
-2	1010	982
-1	425	425
H=	4, K=	-5
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1	711	713
2	145	-161
3	874	-828
4	520	-496
5	252	-250
6	103	96
7	108	122
8	615	-610
9	387	-389
10	482	488
11	114	103
12	-63	-46
13	196	-172
14	144	146
15	197	200
16	269	262
17	133	-114
-15	146	-165
-14	-68	23
-13	283	256
-12	119	-100
-11	294	-294
-10	283	-285
-9	-62	33
-8	426	439
-7	187	-156
-6	647	-642
-5	101	-15
-4	782	736
-3	691	612
-2	117	77
-1	870	-796
H=	4, K=	-4
0	439	447
1	940	-861
2	1176	-1074
3	829	779
4	254	282
5	216	-216
6	641	-636
7	152	-163
8	645	634
9	442	439
10	233	-226
11	178	-198
12	-64	-60
13	101	78
14	120	106
15	258	-256
16	283	-245
-16	-66	0
-15	196	189
-14	-65	10
-13	309	-304
-12	-65	-35
-11	359	352
-10	365	370
-9	-60	-55
-8	700	-731
-7	428	-385
-6	234	241
-5	466	572
-4	837	-834
-3	968	-1107
-2	148	-205
-1	672	684
H=	4, K=	-3
0	332	-276
1	1215	1101
2	388	393
3	349	-327
4	-55	-52
5	74	10
6	758	725
7	262	284
8	399	-415
9	164	-160
10	236	233
11	345	332

L	FO	FC
12	340	341
13	432	-455
14	448	-458
15	333	336
-17	168	163
-16	-65	-15
-15	256	-258
-14	142	116
-13	317	316
-12	-64	57
-11	138	-172
-10	240	-245
-9	121	112
-8	731	717
-7	224	236
-6	150	-217
-5	130	315
-4	449	462
-3	592	418
-2	177	162
-1	931	-821

H= 4, K= -2

L	FO	FC
0	1117	1036
1	287	-277
2	327	-359
3	1049	939
4	1160	1160
5	445	411
6	499	-477
7	703	-697
8	266	285
9	102	-70
10	223	-233
11	474	-461
12	189	-189
13	217	235
14	265	274
15	169	-164
-18	-67	-69
-17	234	-222
-16	-65	-10
-15	232	239
-14	173	185
-13	210	-232
-12	230	-216
-11	158	134
-10	619	632
-9	164	104
-8	692	-695
-7	-55	11
-6	884	822
-5	519	-231
-4	941	-925
-3	68	-234
-2	797	-754
-1	-54	113

H= 4, K= -1

L	FO	FC
0	382	345
1	804	710
2	392	389
3	230	-255
4	1059	-989
5	-54	-54
6	558	543
7	331	316
8	91	-81
9	119	-118
10	-65	13
11	195	186
12	177	164
13	127	-152
14	-68	-75
-19	-68	-80
-18	-68	81
-17	182	188
-16	-64	-80
-15	134	-136
-14	103	81
-13	221	230
-12	420	441
-11	-56	-33
-10	461	-497
-9	409	418
-8	459	417
-7	173	-199
-6	264	-290
-5	337	471
-4	672	-587
-3	445	-534
-2	751	-583
-1	87	-107

H= 5, K= 0

L	FO	FC
0	-52	-15
1	370	-348
2	866	-850
3	109	118
4	411	394
5	141	137
6	444	-431
7	185	-190
8	275	272
9	243	228
10	169	-179
11	393	-374
12	-71	-7
-20	133	130
-19	101	116
-18	205	-205
-17	-65	-12
-16	386	368
-15	251	245
-14	-62	40
-13	167	-192
-12	378	-407
-11	470	473
-10	793	778
-9	1019	-952
-8	575	-565
-7	472	492
-6	1111	1044
-5	1033	941
-4	680	-624
-3	216	131
-2	514	502
-1	560	606

H= 5, K= 1

L	FO	FC
0	589	-603
1	769	749
2	901	857
3	356	-341
4	352	-346
5	149	189
6	290	318
7	-67	71
8	225	-228
9	269	-272
10	-68	33
11	259	258
-20	204	-202
-19	-66	-27
-18	301	298
-17	-65	44
-16	160	-125
-15	93	-92
-14	88	59
-13	431	432
-12	425	464
-11	573	-544
-10	299	258
-9	716	716
-8	109	-5
-7	89	-80
-6	769	-736
-5	301	-285
-4	759	689
-3	420	374
-2	187	-165
-1	511	-478

H= 5, K= 2

L	FO	FC
0	336	329
1	777	-754
2	582	-575
3	197	188
4	359	367
5	226	-222
6	222	-190
7	-66	-16
8	121	152
9	285	292
10	-69	13
-21	-68	7
-20	301	276
-19	-65	-9
-18	247	-249
-17	96	-86
-16	-64	27
-15	-64	89
-14	203	-183
-13	647	-649
-12	332	-341
-11	285	283
-10	575	549
-9	-54	-80
-8	-52	-107
-7	318	-275
-6	739	716
-5	114	132
-4	787	-788
-3	332	-374
-2	-54	75
-1	573	556

H= 5, K= 3

L	FO	FC
0	258	-264
1	625	598
2	379	382
3	212	-190
4	236	-241
5	133	130
6	144	173
7	232	211
8	-71	-89
-21	-68	-33
-20	221	-229
-19	107	-68
-18	-64	49
-17	-66	63
-16	-65	-84
-15	180	-173
-14	-62	-24
-13	262	262
-12	294	304
-11	279	-277
-10	293	-319
-9	133	90
-8	353	361
-7	334	343
-6	450	-422
-5	144	-176
-4	190	185
-3	298	285
-2	159	-148
-1	327	-327

H= 5, K= 4

L	FO	FC
0	177	-164
1	495	-482
2	-66	-20
3	-68	-15
4	299	296
5	141	153
6	330	-323
7	-72	-108
-21	-68	21
-20	132	102
-19	-64	69
-18	-66	-98
-17	625	-605
-16	-67	-82
-15	315	314
-14	104	-75
-13	269	-286
-12	-58	47
-11	361	357
-10	870	822
-9	198	165
-8	624	-633
-7	120	114
-6	-57	121
-5	106	-128
-4	296	-311
-3	566	-548
-2	199	-204
-1	425	435

H= 5, K= 5

L	FO	FC
0	-67	41
1	263	238
2	205	195
3	-69	-100
4	348	-344
5	-70	9
6	276	286
-21	-67	-34
-20	150	-175
-19	-64	-76
-18	341	334
-17	573	566
-16	170	165
-15	385	-394
-14	-63	20
-13	535	538
-12	-60	-29
-11	444	-421
-10	529	-540
-9	-60	-79
-8	795	776
-7	-59	-5
-6	485	-490
-5	426	-433
-4	337	347
-3	430	417
-2	-64	-55
-1	476	-455

H= 5, K= 6

L	FO	FC
0	-70	-95
1	137	-159
2	178	-167
3	-70	60
4	183	198
-21	98	-85
-20	124	151
-19	118	123
-18	281	-288
-17	451	-447
-16	125	108
-15	648	659

L	FO	FC
-14	109	-86
-13	135	-135
-12	-62	11
-11	120	-90
-10	585	585
-9	-62	-41
-8	452	-468
-7	-63	-38
-6	221	202
-5	511	511
-4	-65	35
-3	358	-238
-2	-70	105
-1	464	472

H= 5, K= 7

L	FO	FC
0	204	-196
1	107	96
2	165	176
-21	127	102
-20	131	-127
-19	159	-164
-18	245	250
-17	332	319
-16	221	-208
-15	628	-643
-14	223	-203
-13	107	118
-12	365	345
-11	-65	10
-10	561	-558
-9	141	116
-8	307	309
-7	190	167
-6	-66	30
-5	278	-265
-4	210	196
-3	438	426
-2	-69	-82
-1	333	-334

H= 5, K= 8

L	FO	FC
0	-71	81
-21	179	-162
-20	218	214
-19	175	156
-18	-66	-86
-17	98	-95
-16	-65	-91
-15	289	293
-14	189	214
-13	235	-230
-12	293	-307
-11	-68	119
-10	434	448
-9	-67	19
-8	134	160
-7	304	-314
-6	101	-71
-5	218	188
-4	-65	-33
-3	-69	-119
-2	-68	-60
-1	-68	-16

H= 5, K= 9

L	FO	FC
-20	279	-276
-19	122	-136
-18	-67	22
-17	-66	-84
-16	-67	-98
-15	253	-247
-14	210	-219
-13	177	178
-12	354	337
-11	128	-145
-10	288	-280
-9	170	-159
-8	199	224
-7	329	330
-6	231	-246
-5	251	-253
-4	113	98
-3	112	117
-2	-72	-34

H= 5, K= 10

L	FO	FC
-19	178	168
-18	-68	-28
-17	128	-159
-16	-66	2
-15	217	217
-14	168	183
-13	146	-131
-12	229	-243
-11	-69	54
-10	204	217
-9	-69	-24
-8	134	-153
-7	-70	-43
-6	118	145
-5	235	240

H= 5, K= 11

L	FO	FC
-17	163	175
-16	111	124
-15	273	-274
-14	110	-111
-13	276	261
-12	143	166
-11	-71	-121
-10	-73	-115
-9	-72	-78

H= 5, K= -15

L	FO	FC
7	188	-190
8	141	-111
9	116	92

H= 5, K= -14

L	FO	FC
1	169	-174
2	-69	-26
3	319	312
4	121	108
5	253	-245
6	183	-168
7	-68	81
8	340	392
9	141	129
10	283	-261
11	-67	-83
12	203	208
13	127	117

H= 5, K= -13

L	FO	FC
0	121	100
1	127	124
2	-66	6
3	165	-166
4	-67	-5
5	-63	53
6	147	123
7	-67	100
8	301	-289
9	-65	-68
10	190	190
11	121	112
12	213	-215
13	225	-250
14	-68	54
-2	-68	-44
-1	-70	-123

H= 5, K= -12

L	FO	FC
0	-65	28
1	322	-335
2	-66	-62
3	293	296
4	132	114
5	155	137
6	279	-286
7	-64	-36
8	107	103
9	179	-207
10	303	-302
11	144	-120
12	-67	106
13	405	381
14	124	118
15	250	-232
-4	194	-180
-3	191	-202
-2	-69	121
-1	368	378

H= 5, K= -11

L	FO	FC
0	-65	8
1	237	242
2	129	-115
3	271	-261
4	-66	13
5	174	-173
6	-65	-45
7	99	82
8	137	-123
9	107	98
10	-66	43
11	-65	-93
12	-64	-60
13	123	-124
14	112	128
15	273	273
16	-67	-24
-6	121	-110
-5	-68	4
-4	-65	90
-3	126	112
-2	96	-73
-1	185	-207

H= 5, K= -10

L	FO	FC
0	-65	-3
1	404	-447
2	-65	68
3	237	269
4	119	122
5	-63	-9
6	604	-605
7	165	155
8	611	608
9	-66	79
10	198	-204
11	103	-98
12	277	271
13	151	138
14	329	-341
15	327	-351
16	-66	66
-8	239	-240
-7	119	105
-6	234	243
-5	-64	-11
-4	125	-141
-3	100	-84
-2	396	383
-1	430	422

H= 5, K= -9

L	FO	FC
0	109	106
1	286	287
2	-59	25
3	-59	-35
4	310	-290
5	430	444
6	333	316
7	266	-284
8	422	-426
9	-63	-32
10	173	162
11	181	194
12	140	-163
13	278	-293
14	212	225
15	269	278
16	-66	50
-10	-71	47
-9	348	356
-8	191	204
-7	229	-231
-6	196	-184
-5	-65	-12
-4	240	256
-3	239	212
-2	283	-291
-1	160	-148

H= 5, K= -8

L	FO	FC
0	-59	-76
1	545	-544
2	335	-309
3	584	594
4	363	379
5	526	-522
6	272	-291
7	133	125
8	357	354
9	221	201
10	111	-130
11	209	-220
12	103	129
13	224	235
14	126	-99
15	299	-301
16	220	-203
-11	138	166
-10	136	110
-9	378	-381
-8	257	-281
-7	-64	-38
-6	184	198
-5	-65	6
-4	577	-575
-3	225	-238
-2	413	423
-1	576	542

H= 5, K= -7

L	FO	FC
0	128	126
1	414	378
2	926	897
3	525	-509
4	242	-229
5	653	632
6	-56	18
7	117	-120
8	222	-207
9	357	-336
10	198	215

L	FO	FC
11	340	336
12	-65	-71
13	105	-125
14	-64	67
15	160	167
16	250	253
-13	109	148
-12	174	174
-11	362	-351
-10	225	-221
-9	120	106
-8	-66	65
-7	-64	-14
-6	349	-354
-5	191	-164
-4	533	560
-3	-59	-18
-2	669	-631
-1	108	-73

H= 5, K= -6

L	FO	FC
0	249	-265
1	732	-733
2	538	-540
3	723	709
4	566	554
5	91	40
6	577	-520
7	-56	18
8	195	181
9	132	-131
10	584	-563
11	421	-414
12	-65	-18
13	175	181
14	125	117
15	170	-201
16	207	-187
-14	-67	17
-13	225	-248
-12	120	-128
-11	150	156
-10	103	88
-9	134	-120
-8	261	-291
-7	-61	13
-6	392	381
-5	109	99
-4	346	-320
-3	139	-115
-2	-54	103
-1	345	334

H= 5, K= -5

L	FO	FC
0	90	127
1	434	414
2	471	428
3	1008	-998
4	1005	-935
5	132	117
6	766	754
7	-58	79
8	592	-571
9	97	-90
10	596	573
11	469	455
12	-65	-122
13	241	-251
14	111	-126
15	276	284
-15	-69	-111
-14	135	128
-13	304	297
-12	119	95
-11	221	-221
-10	-65	94
-9	210	200
-8	283	289
-7	226	-195
-6	337	-364
-5	280	254
-4	117	203
-3	106	145
-2	553	-516
-1	193	-232

H= 5, K= -4

L	FO	FC
0	228	250
1	581	-586
2	594	580
3	1101	1020
4	448	455
5	-54	21
6	513	-526
7	197	-199
8	533	521
9	347	374
10	481	-482
11	341	-330
12	119	122
13	290	295
14	116	110
15	319	-321
-16	-68	42
-15	230	225
-14	236	-228
-13	301	-314
-12	170	181
-11	286	301
-10	173	184
-9	-62	-139
-8	544	-578
-7	-56	64
-6	589	530
-5	128	-169
-4	509	-454
-3	482	-415
-2	818	774
-1	698	632

H= 5, K= -3

L	FO	FC
0	323	312
1	910	925
2	635	-600
3	242	-234
4	374	-380
5	98	96
6	485	491
7	273	278
8	576	-588
9	-63	49
10	450	456
11	170	197
12	-65	-52
13	511	-507
14	134	-124
-17	143	167
-16	212	-199
-15	259	-259
-14	147	160
-13	277	271
-12	-64	11
-11	90	-110
-10	222	-235
-9	-55	54
-8	396	397
-7	250	-225
-6	311	-395
-5	130	-212
-4	362	450
-3	1023	1016
-2	740	-742
-1	1344	-1229

H= 5, K= -2

L	FO	FC
0	-55	6
1	576	-555
2	320	289
3	285	292
4	406	405
5	104	-120
6	659	-663
7	94	-46
8	200	176
9	118	-101
10	-66	-99
11	108	-67
12	-67	-42
13	356	352
-18	-67	-89
-17	300	-296
-16	97	76
-15	412	418
-14	-66	19
-13	320	-349
-12	-61	-27
-11	209	225
-10	534	575
-9	94	-91
-8	490	-514
-7	-51	83
-6	419	316
-5	360	309
-4	568	-467
-3	1213	-1184
-2	-55	-51
-1	1228	1209

H= 5, K= -1

L	FO	FC
0	160	-142
1	444	404
2	601	595
3	369	-350
4	500	-512
5	233	247
6	465	447
7	410	419
8	146	-143
9	310	-338
10	177	155
11	243	236
12	-67	-47
13	297	-296
-19	118	-119
-18	-66	41
-17	133	160
-16	155	-156
-15	117	-102
-14	-64	89
-13	292	279
-12	112	95
-11	461	-422
-10	395	-413
-9	140	-81
-8	470	453
-7	166	-84
-6	398	-452
-5	1193	-1195
-4	-54	7
-3	419	-447
-2	818	-775
-1	440	-415

H= 6, K= 0

L	FO	FC
0	-56	102
1	444	-450
2	330	-323
3	-62	-29
4	-63	26
5	204	-223
6	162	-175
7	-66	76
8	252	267
9	168	149
10	186	-196
-20	178	180
-19	-66	4
-18	294	-286
-17	155	-156
-16	148	144
-15	156	150
-14	145	170
-13	345	-350
-12	166	-191
-11	831	855
-10	-57	62
-9	431	-442
-8	-54	-46
-7	495	-449
-6	482	493
-5	551	527
-4	717	-669
-3	406	-421
-2	830	822
-1	280	279

H= 6, K= 1

L	FO	FC
0	-60	-56
1	501	505
2	-62	-85
3	296	-311
4	123	-101
5	190	173
6	199	[illegible]
7	-66	47
8	312	-319
9	172	-153
-20	206	-191
-19	-67	36
-18	224	245
-17	242	240
-16	201	-167
-15	372	-386
-14	175	-168
-13	542	569
-12	439	-414
-11	305	-264
-10	98	-70
-9	216	-196
-8	531	468
-7	198	165
-6	644	-665
-5	419	-420
-4	737	720
-3	-53	73
-2	334	-331
-1	427	-422

H= 6, K= 2

L	FO	FC
0	-61	-11
1	634	-617
2	206	-190
3	324	314
4	118	137
5	-64	-44
6	149	-144
7	-69	-36
8	376	371
-21	-66	23
-20	165	162
-19	136	-95
-18	326	-319
-17	163	-194

L	FO	FC
-16	176	165
-15	505	518
-14	-63	-67
-13	625	-625
-12	-59	1
-11	292	320
-10	251	253
-9	216	-207
-8	402	-406
-7	-53	-33
-6	572	567
-5	207	183
-4	310	-292
-3	109	71
-2	-59	-89
-1	171	183
H=	6, K=	3
0	-65	40
1	367	365
2	-67	57
3	252	-246
4	220	-206
5	-67	-22
6	300	287
7	-69	1
-21	-65	-11
-20	154	-196
-19	-65	42
-18	216	213
-17	104	75
-16	306	-309
-15	566	-592
-14	-63	-47
-13	433	421
-12	324	319
-11	179	-180
-10	239	-200
-9	251	265
-8	495	475
-7	101	-84
-6	243	-268
-5	439	-424
-4	244	245
-3	311	296
-2	139	-133
-1	462	-475
H=	6, K=	4
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1	247	-226
2	103	-99
3	213	210
4	259	281
5	-71	-77
-21	183	159
-20	201	189
-19	-63	22
-18	152	-151
-17	-64	-37
-16	295	295
-15	510	512
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-13	150	-131
-12	132	-138
-11	288	302
-10	544	566
-9	-62	127
-8	123	-120
-7	112	133
-6	229	239
-5	-62	-40
-4	335	-337
-3	320	-345
-2	-60	50
-1	298	293
H=	6, K=	5
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1	137	158
2	-69	95
3	128	-115
4	163	-172
-21	171	-166
-20	231	-219
-19	116	-80
-18	-66	84
-17	-66	68
-16	239	-223
-15	301	-274
-14	200	193
-13	-64	60
-12	-64	-51
-11	221	-222
-10	674	-668
-9	245	219
-8	556	566
-7	234	-274
-6	182	-182
-5	157	161
-4	224	214
-3	366	364
-2	136	-149
-1	260	-262
H=	6, K=	6
0	-68	56
1	104	-115
2	154	-146
-21	-67	-16
-20	236	214
-19	149	133
-18	97	-131
-17	106	-120
-16	192	184
-15	-66	-17
-14	-66	-54
-13	-68	-149
-12	205	-223
-11	257	267
-10	532	528
-9	274	-259
-8	255	-249
-7	131	129
-6	132	66
-5	135	142
-4	202	-194
-3	363	-366
-2	250	218
-1	130	126
H=	6, K=	7
0	164	-181
-21	-68	45
-20	202	-209
-19	120	-107
-18	270	251
-17	255	257
-16	271	-268
-15	335	-336
-14	-67	-52
-13	502	514
-12	170	172
-11	272	-297
-10	346	-367
-9	299	305
-8	211	224
-7	102	-62
-6	104	-115
-5	395	-376
-4	307	277
-3	483	464
-2	-70	-22
-1	246	-250
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-20	277	265
-19	126	105
-18	143	-152
-17	173	-195
-16	125	-64
-15	351	350
-14	-67	79
-13	425	-430
-12	163	-180
-11	-67	127
-10	158	150
-9	-67	58
-8	375	-393
-7	327	-346
-6	310	322
-5	397	398
-4	112	-105
-3	236	-231
-2	109	-120
H=	6, K=	9
-19	-69	-24
-18	210	199
-17	-68	75
-16	-69	-71
-15	364	-363
-14	-68	-72
-13	390	374
-12	201	200
-11	149	-123
-10	298	-301
-9	126	92
-8	469	483
-7	-74	121
-6	159	-168
-5	199	-179
H=	6, K=	10
-17	149	-123
-16	-71	-31
-15	307	302
-14	-68	40
-13	233	-222
-12	131	-113
-11	-71	67
-10	151	130
-9	-72	63
-8	122	-76
H=	6, K=	-14
1	110	-120
2	179	152
3	277	271
4	-68	-5
5	164	-147
6	-67	-13
7	-67	54
8	221	220
9	-69	-73
10	295	-303
11	-70	58
H=	6, K=	-13
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1	215	214
2	-66	15
3	217	-220
4	-66	-40
5	-66	88
6	-67	54
7	297	-290
8	380	-362
9	196	170
10	272	272
11	-67	-19
12	-68	-98
13	103	-90
-2	161	-154
-1	-69	-23
H=	6, K=	-12
0	131	-122
1	369	-357
2	-66	-25
3	294	294
4	116	113
5	335	-355
6	237	-250
7	127	141
8	209	231
9	117	-105
10	155	-132
11	184	-178
12	-65	-41
13	276	285
14	-67	-12
-5	-73	-99
-4	235	-232
-3	-68	-58
-2	383	370
-1	313	304
H=	6, K=	-11
0	129	115
1	301	311
2	-66	15
3	297	-302
4	144	-128
5	101	88
6	689	684
7	187	169
8	452	-481
9	-65	45
10	-64	54
11	217	226
12	131	103
13	184	-176
14	-67	-43
15	192	133
-7	-73	-151
-6	148	-126
-5	-69	116
-4	150	153
-3	139	143
-2	-66	-73
-1	231	-233
H=	6, K=	-10
0	330	-326
1	308	-320
2	-65	-44
3	173	150
4	466	460
5	179	-155
6	479	-489
7	259	264
8	249	255
9	93	-53
10	174	-140
11	326	-344
12	-64	-30
13	238	250
14	-67	-36

L	FO	FC
15	153	-131
-9	318	-306
-8	122	-88
-7	208	199
-6	136	129
-5	-66	-43
-4	251	-235
-3	-65	15
-2	503	530
-1	227	240

H= 6, K= -9

L	FO	FC
0	192	185
1	205	191
2	-61	60
3	277	-310
4	166	-138
5	249	257
6	130	115
7	129	-151
8	104	-104
9	-64	-14
10	305	291
11	309	321
12	307	-311
13	315	-306
14	190	162
15	138	154
-10	-69	57
-9	155	149
-8	-66	-34
-7	135	-127
-6	209	-208
-5	-65	-25
-4	337	338
-3	-66	-70
-2	460	-479
-1	388	-384

H= 6, K= -8

L	FO	FC
0	247	-232
1	443	-451
2	257	261
3	731	726
4	-60	22
5	429	-402
6	194	-182
7	-60	21
8	272	285
9	132	130
10	545	-571
11	-64	28
12	461	460
13	144	136
14	159	-187
15	167	-196
-12	-70	-52
-11	230	231
-10	-69	-94
-9	269	-273
-8	-65	-48
-7	-65	83
-6	267	264
-5	113	-144
-4	449	-460
-3	141	-146
-2	354	352
-1	290	295

H= 6, K= -7

L	FO	FC
0	192	203
1	657	686
2	155	146
3	481	-512
4	126	93
5	305	326
6	90	94
7	-61	-79
8	603	-604
9	174	-162
10	541	528
11	-64	-6
12	382	-386
13	174	-178
14	-66	69
15	170	176
-13	287	280
-12	-68	-13
-11	347	-363
-10	250	245
-9	235	237
-8	163	150
-7	-66	-11
-6	354	-397
-5	212	-226
-4	133	131
-3	-59	22
-2	330	-312
-1	333	-300

H= 6, K= -6

L	FO	FC
0	-54	-48
1	96	-155
2	-55	-34
3	403	414
4	95	75
5	424	-412
6	-59	0
7	-60	-2
8	195	200
9	-63	-36
10	410	-403
11	163	-174
12	252	248
13	261	264
14	-67	39
-14	-71	-41
-13	272	-272
-12	185	196
-11	483	510
-10	106	119
-9	106	-103
-8	239	-258
-7	95	-67
-6	541	550
-5	-58	26
-4	357	-387
-3	141	-153
-2	640	642
-1	417	440

H= 6, K= -5

L	FO	FC
0	153	119
1	389	400
2	177	-183
3	683	-669
4	280	256
5	549	531
6	286	301
7	-61	8
8	385	-377
9	149	149
10	440	436
11	173	175
12	117	-133
13	170	-179
14	-68	-77
-15	124	-133
-14	172	185
-13	356	363
-12	121	-123
-11	240	-251
-10	481	-501
-9	-65	-103
-8	295	283
-7	712	-642
-6	685	-689
-5	338	301
-4	569	520
-3	361	346
-2	309	-287
-1	321	-329

H= 6, K= -4

L	FO	FC
0	176	-192
1	362	-336
2	-54	-88
3	221	235
4	286	305
5	210	-212
6	468	-457
7	92	46
8	506	507
9	108	-91
10	406	-407
11	-64	-86
12	-67	78
13	232	235
-17	-70	-98
-16	118	126
-15	105	86
-14	215	-211
-13	246	-237
-12	159	-171
-11	-64	39
-10	399	412
-9	398	-375
-8	285	-317
-7	507	546
-6	527	586
-5	212	153
-4	238	-277
-3	-52	-58
-2	-52	81
-1	-52	-2

H= 6, K= -3

L	FO	FC
0	244	270
1	445	436
2	482	460
3	456	-454
4	775	-757
5	216	212
6	779	787
7	349	-354
8	227	-204
9	287	273
10	109	108
11	218	212
12	134	-95
13	424	-403
-17	111	112
-16	219	-216
-15	251	-259
-14	172	204
-13	130	166
-12	221	203
-11	88	-43
-10	215	-238
-9	444	425
-8	183	173
-7	614	-530
-6	173	-127
-5	114	18
-4	310	238
-3	220	235
-2	705	-683
-1	880	-857

H= 6, K= -2

L	FO	FC
0	161	161
1	555	-541
2	544	-513
3	342	342
4	550	546
5	212	-214
6	343	-336
7	-65	58
8	-67	-60
9	229	235
10	-65	-26
11	253	-244
12	-69	18
-18	177	-175
-17	258	-274
-16	220	239
-15	380	371
-14	291	-269
-13	-64	-8.
-12	-63	-127
-11	432	447
-10	355	355
-9	-55	-32
-8	-54	-112
-7	-53	106
-6	-52	-10
-5	257	-258
-4	738	-695
-3	1030	-966
-2	-51	-11
-1	385	374

H= 6, K= -1

L	FO	FC
0	288	300
1	1014	976
2	553	536
3	-59	-95
4	-60	19
5	231	206
6	343	333
7	-65	25
8	408	-399
9	177	-184
10	122	117
11	-71	108
-19	97	-78
-18	102	126
-17	245	242
-16	105	-107
-15	-65	-51
-14	145	169
-13	158	186
-12	305	301
-11	404	-391
-10	540	-530
-9	493	470
-8	913	864
-7	-53	18
-6	418	-416
-5	-52	-40
-4	467	521
-3	331	356
-2	402	-411
-1	498	-483

H= 7, K= 0

L	FO	FC
0	262	228
1	490	-487
2	201	-205
3	201	189
4	-65	-60
5	196	-195

L	FO	FC
6	-66	-59
7	190	170
8	273	280
-19	159	-155
-18	164	-150
-17	128	173
-16	404	404
-15	247	247
-14	-65	47
-13	425	-407
-12	-62	-21
-11	145	145
-10	-59	-66
-9	159	156
-8	421	-382
-7	197	191
-6	390	416
-5	-56	-112
-4	708	-700
-3	128	-111
-2	203	180
-1	150	143
H=	7, K=	1
0	-63	-53
1	286	272
2	-69	-152
3	235	-224
4	120	140
5	-64	81
6	161	172
7	-70	-95
-20	183	-173
-19	104	84
-18	144	135
-17	144	-157
-16	171	-155
-15	370	-370
-14	185	169
-13	309	307
-12	-63	-62
-11	140	-146
-10	476	-498
-9	168	188
-8	452	469
-7	383	-365
-6	379	-397
-5	391	378
-4	478	482
-3	166	-134
-2	198	-191
-1	203	-211
H=	7, K=	2
0	114	-93
1	328	-338
2	130	131
3	183	190
4	-65	47
5	-66	-2
6	207	-209
-20	260	234
-19	-64	25
-18	-66	-40
-17	-65	-53
-16	-65	8
-15	363	355
-14	340	-347
-13	301	-272
-12	-62	47
-11	356	370
-10	436	404
-9	114	-97
-8	393	-375
-7	231	219
-6	423	411

L	FO	FC
-5	-61	36
-4	-62	-69
-3	180	-158
-2	-64	-53
-1	236	219
H=	7, K=	3
0	-67	53
1	273	269
2	-65	-40
3	246	-237
4	224	-218
5	-70	65
-21	-69	-84
-20	227	-249
-19	110	-83
-18	115	118
-17	143	161
-16	-66	-66
-15	316	-320
-14	225	234
-13	414	410
-12	-63	34
-11	165	-175
-10	-62	-4
-9	444	435
-8	330	328
-7	164	146
-6	439	-439
-5	155	-148
-4	364	354
-3	157	217
-2	-66	-7
-1	224	-215
H=	7, K=	4
0	153	-142
1	178	-159
2	-69	10
3	130	147
-21	-68	45
-20	104	98
-19	-65	40
-18	205	-207
-17	391	-404
-16	177	189
-15	126	126
-14	278	-275
-13	247	-226
-12	105	-73
-11	207	128
-10	147	111
-9	215	-212
-8	245	-252
-7	174	170
-6	133	109
-5	-66	-90
-4	234	-216
-3	528	-524
-2	175	136
-1	395	412
H=	7, K=	5
0	-68	-30
1	-68	49
2	138	118
-21	-69	-22
-20	178	-187
-19	-64	-27
-18	179	207
-17	228	236
-16	237	-236
-15	-64	-60
-14	-65	-5
-13	257	228

L	FO	FC
-12	118	106
-11	278	-280
-10	140	-105
-9	260	285
-8	216	219
-7	199	-193
-6	152	-141
-5	-67	-71
-4	424	419
-3	428	433
-2	344	-348
-1	204	-211
H=	7, K=	6
0	-71	-11
-20	205	177
-19	-67	74
-18	220	-223
-17	-67	-60
-16	226	223
-15	-66	66
-14	95	42
-13	323	-330
-12	175	-143
-11	231	242
-10	106	133
-9	-68	-103
-8	242	-246
-7	103	120
-6	115	88
-5	-68	84
-4	402	-394
-3	193	-196
-2	386	360
-1	211	180
H=	7, K=	7
-20	218	-202
-19	-68	-10
-18	426	421
-17	-68	-22
-16	187	-181
-15	194	-199
-14	-66	76
-13	297	309
-12	-67	-24
-11	279	-275
-10	172	-169
-9	107	122
-8	190	183
-7	-66	29
-6	143	-176
-5	-70	-70
-4	375	368
-3	122	155
-2	235	-241
H=	7, K=	8
-19	-67	24
-18	156	-148
-17	105	-109
-16	-68	-69
-15	277	265
-14	-68	-38
-13	301	-293
-12	-67	34
-11	197	174
-10	190	176
-9	185	-182
-8	346	-322
-7	151	171
-6	232	261
-5	119	113
H=	7, K=	9

L	FO	FC
-17	-67	13
-16	-70	-75
-15	319	-322
-14	-69	36
-13	258	248
-12	-71	-35
-11	-69	-79
-10	-71	-44
-9	232	249
H=	7, K=	-14
2	-71	110
3	216	198
4	-70	-71
5	-70	-131
6	114	-120
7	140	125
8	258	248
9	155	-156
H=	7, K=	-13
0	215	214
1	191	187
2	177	-171
3	229	-239
4	-65	-22
5	122	134
6	-67	68
7	142	-158
8	178	-159
9	191	187
10	349	355
11	-69	50
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-1	-69	-19
H=	7, K=	-12
0	276	-297
1	129	-134
2	201	224
3	260	265
4	-65	75
5	116	-119
6	-66	-84
7	-64	28
8	230	238
9	101	-55
10	275	-285
11	174	-170
12	305	295
-5	117	-116
-4	203	-180
-3	-69	49
-2	261	247
-1	132	136
H=	7, K=	-11
0	320	309
1	166	169
2	315	-288
3	169	-195
4	152	174
5	611	610
6	265	249
7	520	-537
8	266	-268
9	-67	114
10	-65	112
11	-64	2
12	205	-202
13	237	-243
-7	218	-170
-6	-70	-58

L	FO	FC
-5	-66	0
-4	109	88
-3	-68	75
-2	297	-309
-1	146	-142
H=	7, K=	-10
0	210	-237
1	110	-86
2	-64	47
3	219	215
4	142	-138
5	765	-782
6	151	-120
7	320	344
8	127	131
9	-62	-58
10	201	-193
11	-64	-27
12	325	331
13	222	227
-9	190	-170
-8	-69	11
-7	137	138
-6	130	89
-5	-66	-87
-4	267	-268
-3	-65	51
-2	343	349
-1	149	137
H=	7, K=	-9
0	141	119
1	-64	92
2	-64	70
3	342	-359
4	-64	-2
5	400	399
6	204	216
7	141	-139
8	116	-106
9	-63	92
10	343	356
11	-65	-37
12	385	-402
13	132	-145
-10	-67	10
-9	145	167
-8	-64	13
-7	228	-223
-6	290	-308
-5	108	123
-4	272	272
-3	99	-96
-2	408	-402
-1	-63	-27
H=	7, K=	-8
0	108	-101
1	216	-235
2	106	-78
3	193	187
4	116	116
5	123	-84
6	138	-141
7	94	87
8	347	379
9	-65	-138
10	236	-243
11	-63	42
12	-66	95
13	-66	69
-12	-70	90
-11	273	288
-10	-66	-23

L	FO	FC
-9	100	-144
-8	-65	-63
-7	232	239
-6	238	273
-5	217	-241
-4	235	-219
-3	243	241
-2	233	237
-1	162	150
H=	7, K=	-7
0	171	186
1	554	556
2	257	256
3	259	-255
4	-62	74
5	263	277
6	-63	30
7	200	-209
8	404	-401
9	-63	64
10	237	235
11	-63	18
12	143	-137
13	98	-28
-13	309	311
-12	117	-137
-11	94	-116
-10	-65	46
-9	-64	69
-8	103	75
-7	170	-149
-6	514	-513
-5	163	176
-4	518	520
-3	-62	-95
-2	169	-164
-1	-61	-81
H=	7, K=	-6
0	285	-286
1	607	-626
2	138	129
3	485	477
4	-60	-46
5	251	-248
6	-63	-55
7	144	122
8	313	315
9	140	-153
10	280	-277
11	-64	67
12	194	180
13	-68	92
-14	204	-207
-13	212	-200
-12	188	170
-11	-64	-9
-10	-57	-73
-9	-67	-70
-8	245	-251
-7	240	217
-6	278	272
-5	356	-336
-4	443	-423
-3	303	-314
-2	159	-121
-1	246	250
H=	7, K=	-5
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1	433	424
2	322	-333
3	238	-231
4	155	136

L	FO	FC
5	323	323
6	234	246
7	280	-298
8	339	-331
9	-66	100
10	313	318
11	-64	-32
12	-69	-110
-16	127	-125
-15	121	-120
-14	194	194
-13	-65	27
-12	229	-235
-11	261	-275
-10	168	-166
-9	299	318
-8	-62	-20
-7	294	-323
-6	99	73
-5	173	176
-4	488	503
-3	347	340
-2	421	-397
-1	372	-357
H=	7, K=	-4
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1	294	-273
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3	103	123
4	91	84
5	130	-118
6	220	-222
7	128	155
6	269	266
9	122	-84
10	254	-253
11	-67	-78
12	145	163
-17	133	-117
-16	116	85
-15	201	190
-14	241	-251
-13	121	-119
-12	128	128.
-11	591	600
-10	347	352
-9	293	-247
-8	113	-119
-7	172	125
-6	318	317
-5	152	-122
-4	518	-535
-3	377	-394
-2	88	128
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H=	7, K=	-3
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3	345	-337
4	274	-264
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6	133	116
7	139	-113
8	-64	-5
9	110	-113
10	270	264
11	222	213
-17	134	101
-16	362	-350
-15	264	-276
-14	374	374
-13	307	337
-12	253	262

L	FO	FC
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-10	185	-207
-9	593	627
-8	207	204
-7	-57	-110
-6	540	-506
-5	184	-183
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-3	381	361
-2	1056	-1004
-1	198	-186
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1	143	-150
2	142	-147
3	440	469
4	427	422
5	292	-292
6	138	-156
7	-66	85
8	407	429
9	125	110
10	207	-217
-18	340	-341
-17	164	-190
-16	486	495
-15	355	338
-14	-65	-40
-13	166	-173
-12	179	-172
-11	481	457
-10	355	353
-9	626	-598
-8	641	-594
-7	-57	29
-6	493	471
-5	532	500
-4	228	-254
-3	585	-567
-2	357	374
-1	593	595
H=	7, K=	-1
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2	334	315
3	520	-533
4	129	-104
5	390	397
6	152	145
7	316	-327
8	358	-377
9	-67	-21
-19	-67	42
-18	208	219
-17	-66	-15
-16	456	-441
-15	283	-275
-14	-65	-63
-13	259	274
-12	-63	-58
-11	661	-641
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-9	802	808
-8	227	234
-7	174	-158
-6	315	-328
-5	171	-170
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-3	107	103
-2	454	-468
-1	221	-216

L	FO	FC
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1	229	-237
2	-66	90
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6	260	-251
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-18	170	-147
-17	-64	-11
-16	118	117
-15	367	371
-14	-66	-46
-13	432	-415
-12	-65	-67
-11	151	138
-10	108	-63
-9	329	-332
-8	286	-302
-7	-62	63
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-5	-60	29
-4	461	-482
-3	111	-127
-2	261	256
-1	336	342
H=	8, K=	1
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1	290	286
2	199	-196
3	251	-262
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-19	133	132
-18	168	146
-17	219	205
-16	163	-199
-15	345	-342
-14	364	344
-13	197	187
-12	124	-123
-11	-63	-16
-10	88	24
-9	218	222
-8	268	256
-7	128	-141
-6	90	-98
-5	311	281
-4	436	423
-3	267	241
-2	189	-197
-1	423	-427
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3	201	188
4	101	90
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-19	-66	-63
-18	228	-231
-17	255	-252
-16	225	243
-15	-63	17
-14	284	-271
-13	271	-257
-12	-65	88
-11	109	53
-10	218	223
-9	167	-185
-8	262	-251

L	FO	FC
-7	470	467
-6	360	365
-5	156	-163
-4	396	-408
-3	-67	-61
-2	359	349
-1	383	370
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-19	-67	6
-18	208	187
-17	-66	58
-16	196	-185
-15	-66	-103
-14	192	185
-13	174	162
-12	-66	-82
-11	295	-271
-10	217	-201
-9	284	287
-8	270	249
-7	398	-409
-6	322	-328
-5	284	282
-4	157	144
-3	-66	38
-2	371	-370
-1	327	-323
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-18	271	-262
-17	-65	-55
-16	113	76
-15	-65	-4
-14	-64	-72
-13	134	-139
-12	-65	9
-11	342	346
-10	-66	90
-9	269	-239
-8	-64	-46
-7	234	228
-6	-65	64
-5	-66	-59
-4	132	-120
-3	129	-134
-2	348	364
-1	-67	11
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-19	-66	-19
-18	273	272
-17	-65	74
-16	-65	-49
-15	185	-179
-14	-64	30
-13	151	153
-12	-64	22
-11	213	-232
-10	-64	18
-9	266	255
-8	116	140
-7	155	-170
-6	172	-187
-5	-67	-72

L	FO	FC
-4	-67	91
-3	111	101
-2	118	-100
-1	-67	-16
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-18	253	-266
-17	155	155
-16	156	165
-15	123	152
-14	-64	16
-13	270	-279
-12	-65	-58
-11	196	167
-10	-66	0
-9	136	-138
-8	99	-89
-7	-65	60
-6	220	236
-5	120	138
-4	177	-177
-3	-69	1
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-17	-69	-43
-16	241	-212
-15	271	-272
-14	-66	12
-13	295	293
-12	-67	10
-11	241	-222
-10	-67	-66
-9	-67	59
-8	210	222
-7	-70	-64
-6	259	-258
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-14	131	-140
-13	262	-264
-12	108	141
-11	162	122
-10	-70	21
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5	159	-157
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1	-69	23
2	154	-177
3	-65	8
4	-67	72
5	237	230
6	-68	-48
7	226	-216
8	-70	-80
9	296	273
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H=	8, K=	-12
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2	-65	31
3	271	251
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5	395	-397
6	213	-187

L	FO	FC
7	218	230
8	146	151
9	172	-148
10	150	-126
11	-68	78
-4	205	-212
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-2	327	321
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H=	8, K=	-11
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2	158	-155
3	152	-192
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5	306	309
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7	272	-263
8	132	-120
9	113	92
10	124	118
11	-68	-49
-7	151	-166
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-5	-68	81
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-3	-67	59
-2	-68	-147
-1	-66	7
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1	137	-111
2	232	-229
3	170	192
4	106	-116
5	113	-113
6	151	142
7	210	228
8	133	126
9	108	-95
10	186	-165
11	-68	43
12	374	386
-8	-69	73
-7	-67	87
-6	-65	41
-5	-64	-3
-4	160	-164
-3	-63	27
-2	220	227
-1	129	-121
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2	211	-218
3	-67	-60
4	484	471
5	379	363
6	114	-127
7	202	-192
8	-62	-51
9	-66	95
10	174	168
11	125	-134
12	320	-325
-10	-65	52
-9	144	143
-8	-66	-5
-7	-66	-20
-6	-64	-2
-5	122	132
-4	257	263

L	FO	FC
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-2	278	-268
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H=	8, K=	-8
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1	277	-278
2	570	578
3	274	264
4	216	-244
5	357	-348
6	-64	-26
7	277	280
8	238	247
9	-65	-77
10	277	-276
11	-67	15
12	220	209
-12	156	167
-11	155	168
-10	-65	0
-9	-68	-122
-8	-64	-62
-7	-63	30
-6	-66	101
-5	151	-161
-4	313	-321
-3	-64	-33
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-1	146	139
H=	8, K=	-7
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1	478	485
2	514	-511
3	294	-282
4	137	-125
5	-66	102
6	126	136
7	271	-292
8	444	-440
9	-66	53
10	423	429
11	-67	-12
-13	111	111
-12	154	-151
-11	171	-167
-10	-63	36
-9	170	182
-8	192	185
-7	347	-363
-6	467	-467
-5	212	224
-4	-64	59
-3	204	-195
-2	145	-149
-1	160	-165
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2	173	163
3	297	301
4	268	288
5	132	-139
6	198	-136
7	289	276
8	284	281
9	-67	-91
10	242	-238
11	-66	2
-14	195	-208
-13	-69	-106
-12	109	106
-11	152	163

L	FO	FC
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-9	256	-258
-8	225	-193
-7	363	350
-6	134	134
-5	215	-243
-4	259	-229
-3	-63	-71
-2	239	209
-1	89	133
H=	8, K=	-5
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2	96	-95
3	403	-407
4	-65	-139
5	324	336
6	-64	28
7	333	-338
8	247	-238
9	177	190
10	-67	89
11	99	17
-15	119	-91
-14	212	201
-13	146	128
-12	-64	-19
-11	-65	-19
-10	-66	59
-9	340	338
-8	-64	11
-7	487	-464
-6	191	-203
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-4	476	494
-3	118	99
-2	-60	7
-1	279	-271
H=	8, K=	-4
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1	222	-217
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3	505	505
4	-65	68
5	261	-267
6	-65	24
7	314	315
8	156	134
9	216	-216
10	-68	-97
-16	288	292
-15	-66	31
-14	-64	-81
-13	-64	-25
-12	117	160
-11	144	114
-10	-64	44
-9	461	-447
-8	-65	-35
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-6	411	396
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-4	359	-352
-3	161	-148
-2	317	313
-1	174	150
H=	8, K=	-3
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1	156	138
2	-63	39
3	325	-325
4	172	-145

L	FO	FC
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6	-66	77
7	131	-124
8	141	-144
9	-68	104
-17	312	-303
-16	294	-297
-15	-66	79
-14	242	236
-13	-64	28
-12	312	-302
-11	428	-409
-10	-64	-73
-9	563	549
-8	-61	43
-7	253	-268
-6	114	-121
-5	178	196
-4	727	719
-3	255	-262
-2	875	-887
-1	-60	20
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1	170	-186
2	95	-34
3	510	507
4	180	-178
5	413	-413
6	106	-51
7	184	180
8	210	203
-18	224	-203
-17	-69	79
-16	158	156
-15	-64	-29
-14	402	-412
-13	268	-302
-12	274	249
-11	642	658
-10	-63	9
-9	692	-704
-8	-60	-34
-7	116	123
-6	343	323
-5	-59	-54
-4	826	-814
-3	191	-232
-2	569	594
-1	-61	0
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2	269	-279
3	263	-276
4	158	180
5	140	157
6	-68	121
7	140	-114
8	254	-254
-19	-71	77
-18	126	143
-17	-64	2
-16	136	-126
-15	167	-134
-14	437	439
-13	253	254
-12	117	-115
-11	323	-319
-10	434	447
-9	604	607
-8	238	230
-7	174	-180
-6	494	-454

L	FO	FC
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-4	244	223
-3	-60	0
-2	305	-294
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H=	9, K=	0
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1	199	-198
2	102	105
3	299	315
4	-68	-18
-18	-67	-33
-17	-66	-6
-16	169	155
-15	-66	133
-14	413	-412
-13	368	-343
-12	254	221
-11	227	220
-10	96	-113
-9	214	-201
-8	-65	-53
-7	458	463
-6	303	295
-5	373	-364
-4	-66	57
-3	349	334
-2	296	293
-1	-66	29
H=	9, K=	1
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1	225	189
2	179	-176
3	257	-254
-19	-68	34
-18	138	134
-17	-67	34
-16	418	-442
-15	-64	-24
-14	172	167
-13	-64	-43
-12	201	-194
-11	154	-165
-10	103	37
-9	367	364
-8	269	266
-7	412	-438
-6	186	-175
-5	-67	32
-4	-68	-81
-3	-66	61
-2	275	-280
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1	232	-226
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-18	274	-294
-17	-66	26
-16	264	241
-15	104	91
-14	166	-164
-13	150	-131
-12	114	124
-11	168	159
-10	-66	67
-9	459	-455
-8	-66	-85
-7	452	459
-6	226	227
-5	-66	25
-4	-66	-89

L	FO	FC
-3	244	-257
-2	263	246
-1	-68	33
H=	9, K=	3
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-19	-69	52
-18	248	258
-17	-66	-42
-16	169	-187
-15	150	-146
-14	230	213
-13	248	266
-12	-64	-83
-11	233	-224
-10	102	-69
-9	182	236
-8	-65	52
-7	203	-224
-6	254	-258
-5	109	-89
-4	352	353
-3	219	224
-2	277	-285
-1	100	-75
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-18	264	-273
-17	-68	7
-16	177	165
-15	152	140
-14	249	-245
-13	242	-262
-12	-64	85
-11	229	249
-10	192	175
-9	-68	-121
-8	-65	-8
-7	173	178
-6	196	200
-5	-66	16
-4	383	-395
-3	102	-98
-2	171	172
H=	9, K=	5
-18	276	280
-17	-68	27
-16	165	-155
-15	118	-91
-14	162	157
-13	278	288
-12	-67	-60
-11	375	-373
-10	-66	-4
-9	215	214
-8	-68	62
-7	137	-123
-6	251	-249
-5	-69	28
-4	315	301
H=	9, K=	6
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-16	-68	18
-15	-67	49
-14	160	-152
-13	232	-247
-12	113	111
-11	248	253
-10	107	-81
-9	178	-148
-8	186	-165

L	FO	FC
-7	-71	84
H=	9, K=	-13
0	186	201
1	-69	-51
2	-68	-21
3	203	-176
4	150	129
5	191	192
6	-68	-18
H=	9, K=	-12
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1	-65	-14
2	317	301
3	185	169
4	314	-294
5	205	-231
6	103	81
7	164	161
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-3	140	155
-2	245	245
-1	-68	-106
H=	9, K=	-11
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1	159	-131
2	214	-214
3	-63	-15
4	220	207
5	242	222
6	-68	-109
7	220	-210
8	-66	-54
9	115	120
-6	-67	-12
-5	-68	75
-4	197	189
-3	114	-148
-2	239	-261
-1	144	124
H=	9, K=	-10
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1	274	-273
2	214	203
3	424	420
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5	274	-267
6	-68	66
7	252	251
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9	127	-136
10	209	-191
-8	-68	-3
-7	-67	90
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-5	159	-138
-4	323	-339
-3	181	170
-2	185	194
-1	-66	-133
H=	9, K=	-9
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1	233	235
2	180	-201
3	263	-278
4	-64	-20
5	199	181
6	-62	-22
7	205	-195

L	FO	FC
8	145	-146
9	136	131
10	205	214
-10	112	111
-9	136	151
-8	-67	-20
-7	175	-173
-6	219	-231
-5	-66	127
-4	145	162
-3	222	-227
-2	-64	50
-1	-64	-31
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2	166	158
3	-65	7
4	160	-142
5	184	-175
6	-62	-17
7	376	400
8	202	203
9	215	-219
10	158	-186
-11	145	126
-10	-67	-78
-9	185	-217
-8	-65	-24
-7	226	232
-6	165	177
-5	281	-289
-4	-65	-111
-3	126	128
-2	139	123
-1	113	79
H=	9, K=	-7
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1	202	-201
2	312	-306
3	124	-120
4	170	174
5	285	319
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7	319	-308
8	113	-126
9	254	239
-13	-68	52
-12	153	-146
-11	-65	-82
-10	102	118
-9	184	174
-8	-64	-19
-7	407	-405
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-5	338	334
-4	139	160
-3	-65	-69
-2	292	-280
-1	-64	-46
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2	477	489
3	344	354
4	-66	-50
5	213	-230
6	-64	-10
7	144	119
8	-68	66
9	194	-195
-14	227	-221

L	FO	FC
-13	-67	-34
-12	134	159
-11	-64	61
-10	-64	0
-9	126	-146
-8	-65	-20
-7	382	412
-6	117	76
-5	-66	-161
-4	145	-173
-3	-64	-37
-2	315	320
-1	-65	-68
H=	9, K=	-5
0	372	381
1	251	249
2	324	-317
3	345	-326
4	-64	-34
5	221	218
6	91	87
7	209	-201
8	144	-122
9	122	126
-15	-67	73
-14	121	133
-13	-65	60
-12	190	-168
-11	135	-141
-10	136	169
-9	392	373
-8	-66	-9
-7	334	-350
-6	141	155
-5	117	65
-4	195	186
-3	237	256
-2	524	-532
-1	122	-119
H=	9, K=	-4
0	221	-209
1	305	-303
2	214	225
3	267	265
4	-66	117
5	308	-296
6	161	-171
7	270	234
8	101	138
-16	-68	-8
-15	-69	-35
-14	184	-186
-13	214	-210
-12	188	209
-11	-65	67
-10	185	-205
-9	458	-476
-8	-66	43
-7	375	369
-6	101	-122
-5	-63	-78
-4	356	-358
-3	-64	-56
-2	420	411
-1	201	-199
H=	9, K=	-3
0	100	135
1	219	204
2	158	-143
3	560	-550
4	162	183
5	563	560

L	FO	FC
6	-66	67
7	179	-195
-17	174	-187
-16	-67	-77
-15	-63	-52
-14	152	159
-13	127	107
-12	150	-186
-11	-66	-64
-10	254	250
-9	451	487
-8	188	-172
-7	206	-196
-6	155	-164
-5	244	226
-4	652	646
-3	464	-472
-2	535	-526
-1	-64	16

H= 9, K= -2

0	245	-240
1	218	-227
2	391	383
3	269	280
4	475	-467
5	358	-378
6	-69	-38
-17	-69	120
-16	136	196
-15	-64	67
-14	131	-135
-13	209	199
-12	351	343
-11	109	130
-10	193	-163
-9	284	-338
-8	-64	65
-7	233	226
-6	339	323
-5	411	-430
-4	592	-617
-3	502	497
-2	500	493
-1	210	217

H= 9, K= -1

0	405	394
1	125	112
2	158	-147
3	202	-230
4	123	104
5	363	350
-18	134	110
-17	-67	-46
-16	-64	-13
-15	117	134
-14	121	140
-13	-65	32
-12	179	-184
-11	243	-241
-10	-66	192
-9	264	264
-8	-63	-33
-7	318	-313
-6	164	-146
-5	427	417
-4	310	337
-3	498	-490
-2	402	-396
-1	227	-224

H= 10, K= 0

0	295	-299
1	214	-202

L	FO	FC
2	209	224
-17	-68	-29
-16	231	249
-15	-66	-34
-14	393	-380
-13	-65	-69
-12	196	189
-11	160	155
-10	-63	22
-9	159	-182
-8	-65	-77
-7	357	378
-6	144	128
-5	236	-241
-4	253	-264
-3	-65	-55
-2	331	336
-1	-67	5

H= 10, K= 1

0	269	274
-17	-67	-72
-16	170	-131
-15	282	286
-14	245	252
-13	99	104
-12	212	-225
-11	312	-297
-10	-62	-33
-9	403	414
-8	-66	-6
-7	445	-431
-6	-65	-21
-5	230	226
-4	357	349
-3	-67	-44
-2	271	-273
-1	-67	-28

H= 10, K= 2

-17	181	184
-16	172	178
-15	217	-206
-14	266	-306
-13	97	-89
-12	218	247
-11	298	306
-10	168	-176
-9	420	-404
-8	-68	115
-7	359	333
-6	-66	58
-5	99	-95
-4	318	-308
-3	-68	80
-2	190	184

H= 10, K= 3

-17	176	-174
-16	244	-243
-15	-66	61
-14	208	209
-13	-66	75
-12	245	-250
-11	202	-248
-10	-65	53
-9	348	356
-8	147	146
-7	222	-225
-6	134	-149
-5	114	110
-4	251	248
-3	-70	-15

H= 10, K= 4

L	FO	FC
-16	233	224
-15	-65	28
-14	-69	-125
-13	-68	-112
-12	100	119
-11	287	310
-10	-67	-47
-9	223	-237
-8	-67	-42
-7	-66	51
-6	173	218

H= 10, K= 5

-14	111	101
-13	188	197
-12	209	-201
-11	241	-231
-10	-68	66

H= 10, K= -12

0	138	-106
1	-70	100
2	226	228
3	-69	-10
4	207	-199
-1	-70	-108

H= 10, K= -11

0	-68	79
1	-69	9
2	123	-150
3	184	-174
4	238	219
5	165	167
6	-70	-107
-5	122	124
-4	-69	89
-3	136	-148
-2	142	-137
-1	121	80

H= 10, K= -10

0	279	-282
1	169	-160
2	296	323
3	170	187
4	262	-277
5	-66	-59
6	-67	88
7	-67	-9
-7	113	138
-6	-68	28
-5	170	-199
-4	-67	-72
-3	306	318
-2	-67	82
-1	-65	-48

H= 10, K= -9

0	268	288
1	-64	6
2	360	-363
3	156	-167
4	266	255
5	103	122
6	-67	88
7	127	-100
-9	159	160
-8	-69	4
-7	146	-168
-6	-68	6
-5	342	342

L	FO	FC
-4	-66	43
-3	184	-211
-2	162	-172
-1	-64	-58

H= 10, K= -8

0	362	-360
1	-64	-70
2	328	341
3	256	254
4	-65	-30
5	298	-291
6	-66	-18
7	310	311
-10	159	-159
-9	145	-151
-8	160	138
-7	355	362
-6	-66	-30
-5	272	-266
-4	154	-181
-3	-64	15
-2	253	249
-1	-66	-103

H= 10, K= -7

0	335	360
1	262	261
2	194	-190
3	241	-259
4	-63	23
5	319	319
6	113	67
7	323	-310
-12	153	-130
-11	-66	41
-10	166	145
-9	216	211
-8	-67	-83
-7	426	-441
-6	-67	-103
-5	198	203
-4	94	118
-3	-64	-8
-2	308	-310
-1	-67	136

H= 10, K= -6

0	238	-229
1	-63	-23
2	115	129
3	-63	50
4	-67	-78
5	302	-311
6	-68	-70
7	274	279
-13	96	55
-12	-66	51
-11	125	125
-10	-65	-38
-9	287	-285
-8	-65	38
-7	295	294
-6	-64	-45
-5	179	-201
-4	163	-184
-3	180	154
-2	504	522
-1	-66	-70

H= 10, K= -5

0	220	236
1	138	-159
2	187	-206

L	FO	FC
3	110	-139
4	170	149
5	304	313
6	-67	-70
-14	101	79
-13	-66	55
-12	208	-201
-11	144	-160
-10	-65	89
-9	138	159
-8	-65	-104
-7	320	-323
-6	-64	41
-5	249	262
-4	273	262
-3	371	-290
-2	556	-586
-1	186	175

H= 10, K= -4

L	FO	FC
0	336	-324
1	-64	53
2	195	196
3	293	298
4	171	-165
5	358	-374
6	152	146
-15	-68	-30
-14	-67	-123
-13	-66	-12
-12	281	286
-11	133	124
-10	94	-92
-9	216	-235
-8	156	130
-7	260	248
-6	147	-114
-5	109	20
-4	-66	65
-3	509	517
-2	-66	69
-1	320	-310

H= 10, K= -3

L	FO	FC
0	274	273
1	116	114
2	309	-315
3	279	-273
4	360	374
5	253	274
-16	-66	-35
-15	-66	35
-14	178	187
-13	-65	44
-12	345	-330
-11	-65	-84
-10	257	246
-9	198	194
-8	-64	14
-7	-65	-70
-6	-64	41
-5	238	213
-4	-66	-44
-3	502	-485
-2	110	-125
-1	212	192

H= 10, K= -2

L	FO	FC
0	186	-201
1	133	-101
2	282	285
3	-69	83
4	187	-295
-16	142	112
-15	-66	94

L	FO	FC
-14	-67	-67
-13	-65	-50
-12	172	182
-11	-63	17
-10	161	-205
-9	-64	-64
-8	95	85
-7	227	230
-6	134	141
-5	120	-131
-4	108	-123
-3	111	108
-2	97	106
-1	-64	-48

H= 10, K= -1

L	FO	FC
0	325	337
1	245	242
2	259	-266
3	247	-249
-17	-68	-16
-16	221	-208
-15	267	-282
-14	187	176
-13	148	164
-12	295	-266
-11	-63	-64
-10	146	140
-9	128	111
-8	-64	-26
-7	325	-326
-6	297	-301
-5	233	220
-4	105	110
-3	109	121
-2	281	-267
-1	91	-4

H= 11, K= 0

L	FO	FC
-15	104	-86
-14	208	-185
-13	-66	54
-12	169	175
-11	149	147
-10	117	-127
-9	255	-276
-8	-65	17
-7	277	275
-6	-66	94
-5	127	-112
-4	100	-140
-3	130	129
-2	131	150

H= 11, K= 1

L	FO	FC
-15	-66	28
-14	-67	74
-13	-66	-29
-12	115	-152
-11	263	-254
-10	220	220
-9	257	239
-8	-67	-85
-7	151	-182
-6	-67	-56
-5	130	146
-4	112	144

H= 11, K= 2

L	FO	FC
-15	134	-136
-14	100	-114
-13	110	-113
-12	169	148
-11	243	222

L	FO	FC
-10	189	-188
-9	140	-119
-8	104	109
-7	202	198
-6	-69	61

H= 11, K= 3

L	FO	FC
-13	175	169
-12	192	-215
-11	233	-216
-10	152	153
-9	177	156

H= 11, K= -11

L	FO	FC
0	168	184

H= 11, K= -10

L	FO	FC
0	257	-269
1	-67	-31
2	320	332
3	-69	70
-5	293	-263
-4	-71	-2
-3	340	311
-2	148	147
-1	124	-141

H= 11, K= -9

L	FO	FC
0	263	250
1	-66	30
2	288	-304
3	-66	25
4	220	208
-7	255	-244
-6	-69	106
-5	199	192
-4	147	-116
-3	254	-255
-2	182	-193
-1	140	143

H= 11, K= -8

L	FO	FC
0	287	-287
1	-68	102
2	203	213
3	-65	-35
4	161	-152
-9	144	-133
-8	171	190
-7	123	116
-6	196	-194
-5	152	-147
-4	119	117
-3	307	302
-2	101	117
-1	214	-204

H= 11, K= -7

L	FO	FC
0	358	350
1	148	-147
2	222	-233
3	159	-127
4	-70	81
-11	-69	-91
-10	143	138
-9	216	203
-8	266	-273
-7	210	-216
-6	121	90
-5	126	124
-4	-65	-11
-3	119	-143

L	FO	FC
-2	103	-97
-1	235	256

H= 11, K= -6

L	FO	FC
0	396	-408
1	-66	-29
2	132	121
3	222	236
4	-70	-100
-12	131	140
-11	154	178
-10	262	-240
-9	104	-146
-8	165	160
-7	198	212
-6	127	138
-5	-65	-91
-4	135	-122
-3	-67	90
-2	134	146
-1	245	-244

H= 11, K= -5

L	FO	FC
0	284	276
1	134	135
2	-69	-84
3	195	-183
-13	-67	22
-12	193	-202
-11	125	-115
-10	249	250
-9	141	143
-8	-62	-20
-7	225	-221
-6	-64	-28
-5	98	116
-4	193	212
-3	-64	-23
-2	338	-345
-1	123	97

H= 11, K= -4

L	FO	FC
0	-65	-49
1	-67	9
2	159	162
3	155	126
-14	154	-171
-13	-69	-60
-12	243	241
-11	188	179
-10	130	-119
-9	-63	-55
-8	-64	3
-7	111	161
-6	115	54
-5	140	-141
-4	205	-206
-3	-65	-44
-2	270	264
-1	111	-82

H= 11, K= -3

L	FO	FC
0	-68	-81
1	-67	-31
2	185	-199
-14	175	187
-13	-68	61
-12	302	-307
-11	103	-100
-10	-66	66
-9	-66	115
-8	-64	68
-7	289	-305
-6	100	78

L	FO	FC
-5	430	435
-4	124	155
-3	252	-246
-2	111	-121
-1	210	181

H= 11, K= -2

L	FO	FC
0	160	-174
1	-69	-65
-15	-68	-40
-14	233	-248
-13	-67	-22
-12	285	303
-11	-66	-9
-10	-64	-32
-9	259	-254
-8	-65	-78
-7	271	274
-6	-67	-55
-5	402	-409
-4	-66	-62
-3	199	194
-2	-66	35
-1	-65	7

H= 11, K= -1

L	FO	FC
0	355	352
-15	152	136
-14	377	375
-13	-70	-115
-12	287	-288
-11	-66	-68
-10	-66	94
-9	298	301
-8	-64	-14
-7	301	-288

L	FO	FC
-6	-66	66
-5	167	170
-4	-67	99
-3	-68	-119
-2	222	-204
-1	-68	53

H= 12, K= 0

L	FO	FC
-11	114	114
-10	207	-213
-9	236	-208
-8	101	102

H= 12, K= -8

L	FO	FC
0	172	-199
-6	-68	-25
-5	149	-155
-4	120	-138
-3	-68	98
-2	160	143
-1	194	-181

H= 12, K= -7

L	FO	FC
0	146	122
-8	155	-143
-7	130	-134
-6	-69	60
-5	264	279
-4	119	101
-3	210	-236
-2	132	-119
-1	177	191

H= 12, K= -6

L	FO	FC
0	118	-88
-9	-69	-80
-8	107	103
-7	-68	88
-6	203	-205
-5	346	-371
-4	-67	65
-3	305	309
-2	150	145
-1	197	-216

H= 12, K= -5

L	FO	FC
-11	-67	-38
-10	211	218
-9	-66	15
-8	142	-137
-7	106	-66
-6	142	120
-5	293	287
-4	-69	60
-3	208	-233
-2	117	-157
-1	217	229

H= 12, K= -4

L	FO	FC
-11	-69	-25
-10	226	-235
-9	-66	-75
-8	-65	26
-7	150	176
-6	-67	42
-5	153	-158
-4	103	-65
-3	177	147
-2	111	141
-1	150	-144

L	FO	FC

H= 12, K= -3

L	FO	FC
-12	255	-249
-11	-67	42
-10	141	120
-9	138	150
-8	-67	-34
-7	222	-249
-6	110	84
-5	223	225
-4	-67	23
-3	123	-151
-2	167	-148

H= 12, K= -2

L	FO	FC
-12	-70	132
-11	-66	60
-10	114	-82
-9	183	-201
-8	103	116
-7	270	302
-6	126	-81
-5	210	-219
-4	116	-101

H= 12, K= -1

L	FO	FC
-12	165	-152
-11	97	-103
-10	193	185
-9	201	220
-8	127	-129
-7	213	-214
-6	-67	40

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BIOGRAPHICAL SKETCH

Douglas Allen Sullivan was born November 9, 1945, in Huntington, West Virginia. In May, 1963, he was graduated from Vinson High School, Huntington, West Virginia. He received the degree of Bachelor of Science in Chemistry from Marshall University in May, 1967. After studying at the University of Florida from September, 1967, to August, 1968, Mr. Sullivan taught chemistry, physics, physical science, and mathematics for the Wayne County (West Virginia) Board of Education. He then returned to the University of Florida in September, 1972, and received a Master of Science in Teaching degree majoring in chemistry in December, 1974. He is a member of the American Chemical Society. Mr. Sullivan is married to the former Jeanie Delaine Puckett of Titusville, Florida. They have a three-year-old son, David O'Donald Sullivan.

I certify that I have read this study and that in my opinion it conforms to acceptable standards of scholarly presentation and is fully adequate, in scope and quality, as a dissertation for the degree of Doctor of Philosophy.

Gus J. Palenik

Gus J. Palenik, Chairman
Professor of Chemistry

I certify that I have read this study and that in my opinion it conforms to acceptable standards of scholarly presentation and is fully adequate, in scope and quality, as a dissertation for the degree of Doctor of Philosophy.

R. Carl Stoufer

R. Carl Stoufer
Associate Professor of Chemistry

I certify that I have read this study and that in my opinion it conforms to acceptable standards of scholarly presentation and is fully adequate, in scope and quality, as a dissertation for the degree of Doctor of Philosophy.

G. E. Ryschkewitsch

George E. Ryschkewitsch
Professor of Chemistry

I certify that I have read this study and that in my opinion it conforms to acceptable standards of scholarly presentation and is fully adequate, in scope and quality, as a dissertation for the degree of Doctor of Philosophy.

John F. Helling

John F. Helling
Associate Professor of Chemistry

I certify that I have read this study and that in my opinion it conforms to acceptable standards of scholarly presentation and is fully adequate, in scope and quality, as a dissertation for the degree of Doctor of Philosophy.

Richard R. Renner

Richard R. Renner
Professor of Education

This dissertation was submitted to the Graduate Faculty of the Department of Chemistry in the College of Arts and Sciences and to the Graduate Council, and was was accepted as partial fulfillment of the requirements for the degree of Doctor of Philosophy.

December, 1975

Dean, Graduate School